CompassCDS
Version 4.1.0
Release Notes

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2018
Publication Number BR501489
Revision F

Contents

Contents 2
What's New in CompassCDS 4.1.0 3
CompassCDS Core 3
Control Drivers 3
Add-ons 3
Notes 3
Available Instrument Control Drivers 3
General 6
Notes on CompassCDS Report Editor 11
Notes on CompassCDS Configuration Manager 11
Plug-ins and Add-ons 12

What's New in CompassCDS 4.1.0

CompassCDS Core

Agilent ICF Support – Agilent's Instrument Control Framework (ICF) is now supported and allows to instantly install and use ICF/RC.Net control drivers with the Agilent ICF Driver.

Remote Sequence Manager – Unlike in previous versions the Remote Sequence Manager (External Sequence) is not crashing anymore when executing a sequence. Consequently, with current version the Remote Sequence can be used again in Client/Server environment.

Control Drivers

CompassCDS 4.1.0 supports Agilent's Instrument Control Framework (ICF) and related RC.Net control drivers for Agilent HPLC and GC.

RC.Net control driver for Agilent HPLC

Installer loads control drivers for Agilent HPLC series 1100, 1120 & 1220 Compact, 1200 & 1200 Infinity, 1260 Infinity I, II, and 1290 Infinity II, including fraction collectors and ELSD.

RC.Net control driver for Agilent GC

Installer loads control drivers for Agilent GC series 6890/6850, 7890 A/B, 7820, and 9000 Intuvo including related headspace autosamplers.

Add-ons

CompassCDS AnIML Converter and Viewer

AnIML Converter converts CompassCDS chromatograms into a human readable animl file that can be used for long-term archiving and reviewing of CompassCDS raw data, meta data and results without compromise with the AnIML Viewer component independently of CompassCDS, and also used for extraction and upload of results into LIMS or SAP/ERP.

Notes

Available Instrument Control Drivers

RC.Net Control Drivers

RC.Net control driver for Agilent HPLC

Current version LC Drivers A.02.18

Installer loads control drivers for Agilent HPLC series 1100, 1120 & 1220 Compact, 1200 & 1200 Infinity, 1260 Infinity I, II, and 1290 Infinity II, including fraction collectors (G1364 A/B/C/D, G5664 A, G7159 B, G7166 A), single or clustered. Also, the ELSD models 380/385 (G4260 A & G4261 A), 1260 (G4260 B) and 1290 (G7102 A & G4261 B) are supported.

RC.Net control driver for Agilent GC
Current version GC Drivers B.01.03

Installer loads control drivers for Agilent GC series 6890/6850, 7890 A/B, 7820, and 9000 Intuvo including related headspace autosamplers G4556A (7697A, 11 vials), G4557A (7697A, 111 vials) and G1888A.

Common control drivers

Control Driver for Scion 400 Series GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model 456, 436, 450 and 436 GCs as well as a separate driver for the Varian/Bruker 430 GC.

Control Driver for Varian 3800 Series GC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model Varian 3800 GC.

Control Driver for Varian 3900 Series GC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the model Varian 3900 GC.

Control Driver for Varian SHS-40
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the static SHS-40 headspace autosampler.

Control Driver for CTC CombiPal
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for CTC CombiPAL and xt.

Control Driver for Valco SSV
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Valco SSV.

Control Drivers for NI Devices
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the NI-9181 & NI-9184 chassis as well as drivers for the NI-9219 (Analog data acquisition), NI-9401 (TTL/IO) and NI-9481 (Contact closure relay) module that fit into these chassis.

Analog – Digital data acquisition - NI-9184 4 Slot Chassis fitted with NI-9219 ADC module and also required NI-9401 TTL/IO for inject start input. NI-9481 relay module can be added to this configuration if required. Analog data acquisition is restricted to a single time base with up to 4 channels (detectors) with the current driver.

Contact closure relay control – Either 4 slots NI-9184 or single slot NI-9181 chassis fitted with NI-9481 relay module.

TTL/IO Start in/Start out control - Either 4 slots NI-9184 or single slot NI-9181 chassis fitted with NI-9401 relay module.

Control Driver for Varian STAR 800 & 850 MIB
Current Version: 1.0.0.190

The control driver for the STAR 800 & 850 MIB interface supports analog data acquisition (4 channels), contact closure relay (4), serial (4-8 channels) and GPIB (max 2 IEEE cards) communication.

Control Driver for Agilent 5890 GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 4890 & 5890 Series GCs and associated autosamplers.

Control Driver for Agilent 6890/6850 GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 6890 & 6850 I/II Series GCs and associated autosamplers.

Control Driver for Agilent 7890 A/B GCs
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads a common control driver for the Agilent 7890 A/B Series GCs and associated autosamplers.

Control Driver for Agilent 1260 HPLC
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

This installer loads common control drivers for HP/Agilent 1100, 1200 and 1260 HPLC modules.

Manual Injector
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

Time Control
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

Generic Column Tracker
Current version 4.1.0
Previous version 4.0.1 (CompassCDS 4.0.1)

General

CompassCDS DCOM Tool – A tool for automatically setting all Windows DCOM and folder permissions for client server installations has been created and is included with every CompassCDS DVD. Tool does not replace manual security settings on the CompassCDS\Server and \data folder. For details see the installation guide.

Installation - Before installing CompassCDS, check that the 'File and Printer Sharing for Microsoft Networks' component is installed. This component is listed in the network connections properties. When Internet Explorer 7.0 or Edge is installed on the host computer, at the end of CompassCDS installation, the InstallShield wizard sometimes hangs up and pressing the Finish button does not close the wizard. The only solution is to use Windows task manager and to kill the Setup.exe applications.

It is strongly recommended that the computer be rebooted at the end of the installation.

If the Amyuni PDF driver is failing to install ('spooler error'), locate the file PDFprinter_install.exe in the CompassCDS\client folder and add the –p flag (PDFprinter_install-p.exe) before re-executing the installation. The -p option prevents the install utility from trying to stop and restart the spooler.

If the Amyuni PDF driver is not working then check Windows registry setting. Go to HKEY_CURRENT_CONFIG, then PDF Compatible Printer Driver, Permissions: make sure that "everyone" is set with full control is set. If not, add this to the security settings.

The Configuration Manager audit trail is not automatically archived when uninstalling the software. If you need to recover the audit trail, archive the current audit trail before uninstalling CompassCDS.

Screen Savers and Power Management - It is recommended that all screen savers be disabled. It is better to use the Windows energy saving feature for the monitor. It is recommended that all power management properties be disabled (Standby/Hibernates).

Backup - When backing up CompassCDS files, do not back up the \SERVER directory (including its subdirectories). Doing so will cause the loss of chromatogram files (*.DATA) that were acquired while the backup was being done. It is also recommended to avoid backing up recently acquired CompassCDS Data files (< 5 hours). Backups can only be done if CompassCDS and the Configuration Manager isn't in use and the nexusdb Windows service has been stopped.

Closing the application - Users are also advised not to let a cursor remain within a grid (sequence, identification table, integration table, reprocessing list) when exiting CompassCDS or closing files. If this occurs, the following error message 'Cannot focus a disabled or invisible window' may appear. This message has no consequences, and if it occurs while a sequence is running, the sequence should just be left to terminate before CompassCDS is closed.

Acquisition - If the administrator modifies the configuration of a system in the CompassCDS Configuration Manager (for example, renames a detector, adds or removes a detector, etc.), the methods created before the system configuration modifications will be invalid for acquisition (quick start or sequence). Users will have to create new methods. If the administrator creates, deletes or modifies the name of a system while a user is already connected to a group/project that owns this system, it will be necessary to log in to CompassCDS again to refresh the system list.

Calibration Curve - When working in concentration versus response mode, the format modification functions in the calibration curve table are inverted: when the Quantity variable format is changed, the Area/Height format is changed and when the Area/Height format is changed, the Quantity variable is changed.

Chromatogram - When a sequence or a reprocessing list is open, and the chromatogram data section is displayed and then the sequence (or reprocessing list) is clicked in the browser, the chromatogram trace will not be redisplayed when the chromatogram data section is reselected.

Workaround: click on the method section of the chromatogram and then select the data section to refresh the screen.

Event annotations are not correctly displayed on the chromatogram after extracting an archived data version (get archive option).

Workaround: click on the integration method sub-section to refresh the display.

A calibration curve is created by a user owning the archive calibration curve profile. This curve is cleared and a new point is added by a user that does not own the archive calibration curve profile. Then the user that owns the calibration curve profile reprocesses a chromatogram (F6) with the current curve and then with (F5), the results change because the last archive is used instead of the current one. The workaround is that the last user (archive calibration curve) must save the calibration curve before recalculating the results by (F5).

Suppose a standard chromatogram contains 3 identified and quantified peaks named A, B and C. The user has the 'Use M and D factors for curve building' profile. Peak C is processed as peak A ('Use References' option checked in the calibration table). When both conditions are used, peak C quantity will be Qeq*M/D instead of Qeq (with Qeq: quantity calculated according to the calibration curve equation).

Workaround: create the following variable:

QTY REC: peak user formula, real.

QTY REC = IF((NAME='X');QTY*DIVFACTOR/MULFACTOR;QTY), with X=C in this example.

When the user does not have the right to overwrite data and the data file name already exists, a date/time suffix is automatically added. This timestamp is always displayed with the English date/time format: Month2_Day2_Year4 whatever the regional settings of the PC are.

Electronic Signature - When you have validated your signature in the user identification for sign-off window, press the Close button to exit the window and not the 'X' button in the upper right corner of the window. For this operation, the Windows 'X' button is the same as the Cancel button. If the Windows 'X' button is used, the signature will not be applied. Suppose the user has the batch sign at once profile and a chromatogram has been excluded mistakenly from the list of files to be signed, it is then impossible to sign the corresponding chromatogram.

File Import - If a .CDF file is opened and reprocessed (F6 function) with an external method, no preview is available when selecting the resulting DATA file in the open file window and the absorbance values are null.

Workaround: after opening the .cdf file, save it before reprocessing it.

When importing an AIA file (.CDF) or a Star Workstation chromatogram (.RUN), save it before reintegrating it or reprocessing it.

Method - When printing the control method, a blank page is printed at the end. The control parameters are not printed if you open a chromatogram or a method and then change some method parameters (integration events for instance) before printing.

Workaround: save the method (or chromatogram) before printing.

Only methods created in the project in which the current user is logged are available in the sequence or quick start wizard. If a method created in project 1 is saved as another name in project 2, when logged in project 2 this new method will not be displayed in the sequence and quick start screens.

Method Templates - When creating a new method from template, some acquisition parameters are not imported from the template (run name, run ID, description, vial and rack numbers, injection volume, run length, dead time, specific channel option). Do not uncheck channels or injectors before saving a method as template.

Open File - In the chromatogram open file, only the first line of the run information is displayed in the information field.

PDF Export Plug-In - If the PDF Export plug-in needs to be used with the remote sequence feature, modify the external sequence engine service of the CompassCDS system to run as following:

From Windows, select Start/Control Panel/Administrative Tools/ Services

Locate the service named 'External Sequence engine – SYSTEM_1' (if the CompassCDS system to run is SYSTEM_1).

Right-click on this service and select 'Properties', then select the Log On tab.

Select the ‘This account’ option and select the account information (account name, password and password confirmation) for the account that will be used to start the service. Note that this account should have a default printer defined and a non-blank password.

In the main Services window, right-click on the service that was just modified and stop it so that the changes are taken into account next time the service is started.

Prep-Ahead - Suppose the prep vial number entered in the sequence is N. The real prep vial number taken into account will be N-1.

Using multi-injection per line is not possible in the sequence when working with prep-ahead.

Quick Start - It is not possible to add a summary report (with the add button) from the quick start screen. For multiple injector systems, the export is always performed at the end of the quick start, even though this option has been unchecked in the method properties.

Reprocessing List - If the chromatogram does not contain an acquisition method section (AIA files imported in CompassCDS, etc.), the method name used to reprocess this data will not be automatically imported in the reprocessing list. You must load it manually. The only way to stop a reprocessing list with the bracketing option checked is to close it. The stop button is not available during the calculation step. Do not use the fill block option while the processing list is running. More generally, use the pause option to make any changes when the reprocessing list is running. Assume several chromatograms (A, B, C and D) have been reprocessed with A as a blank and the other ones as standards. Then some of them were modified, the changes were saved, and they were imported into a reprocessing list after sorting them by the modification date in the file open window (for example: D, C, B and A). In the reprocessing list, the files will be displayed in the same order; D, C, B and A, but A will be identified as an unknown instead of a blank. After restoring the initial order (A, B, C and D), redefining the correct sample type for chromatogram A, and running the reprocessing list, it appears that the blank chromatogram subtracted for chromatograms B, C and D is not A.

Reprocessing Single - When manual operation (manual integration or manual identification) has been performed, do not change chromatogram properties (M, D, internal standard quantity, ….) directly from the reprocessing single screen. Firstly, change the required values from the chromatogram itself (by using the chromatogram properties button), then select the reprocessing single option and reprocess the chromatogram. Assume at least two chromatograms (A and B) are opened and are using the internal standard calibration mode. Chromatogram A is selected from the browser. In the reprocessing single window, after selecting chromatogram B and pressing the properties button, it is not possible to enter the internal standard value (the field is grayed out). The workaround is to close the reprocessing window and to select chromatogram B. Then it will be possible to edit the internal standard field directly from the reprocessing window.

Sequence - If a cell in the ‘number of injections’ column (displayed in second position after the ‘Run#’ column) is selected (without putting the cursor in it) and the value 0 is entered, CompassCDS will be frozen. You must end the task to restore CompassCDS operation. Do not use the copy and paste commands to duplicate the calibration cell content. If you select another file in the browser or open another file, an error will appear. The workaround is to use the fill block feature.

On a system with two injectors, if you uncheck one of the injectors and restart the sequence by overwriting the data files, a second injection date (corresponding to the acquisition date of the active

injector) will appear in the run log screen (available in the acquisition sub-section of the chromatogram method). This second date is only displayed for the files that are associated with the injector that is not active.

For multiple-injector systems, select the required sub-system to create fill blocks. When multiple injections are defined per line, if you want to make fill blocks or disable a line:

First, define 1 as number of injections and make the required changes, then enter the desired number of injections.

Otherwise the changes will only be applied on the first injection of the given run.

When several injections are defined per line, do not use the arrows to validate the entries in the No of injections column. It may induce a double numbering of the line index column when printing the sequence.

The processing parameters (pre-processing, integration, identification, calibration…) are disabled in the method properties and are also applied at the end of the acquisition. This is a normal behavior to ensure coherence between the chromatogram method and the results.

When renaming an existing project from the Configuration Manager, the old methods are no longer available from a sequence created before the project is renamed. The workaround is to create a new sequence.

Sequence blank runs - When a sequence that usually starts with line in which the Sample type is defined as a Blank, what happens, is that for all the subsequent runs the blank run is automatically subtracted from each chromatogram. The resulting data-files will all have a line in the pre-processing section, pointing to the blank run. When processed or re-processed the resulting reports show all variables (such as method name, or start run time, username, etc.) as 'not defined' and the peak names are missing from these chromatograms and the results table will be empty. When manually re-processed, these files return a message saying 'processing: aborted'. Only re-processing with the original Global method file resolves this issue, because the line pointing to the sequence blank will be removed.

Workaround: Do not select Sample type Blank if the intention is to first run a blank sample to ensure no sample carry over. Select Sample type Unknown instead.

Star Workstation .RUN file import – Users can once again import legacy Star Workstation .RUN files. CompassCDS will automatically import a copy of the .RUN file and convert it into a .DATA file. Peak names will also be imported.

Summary Report - An extra-printing may occur during the sequence in the following conditions:

The 'print after a new warning' option has been configured.

A warning in the sequence generates the printing of the summary report.

This extra-printing will be performed at the end of each following acquisition only if the chromatogram corresponds to a sample type that is not automatically added into the summary report.

Do not reprocess the same chromatogram several times within a reprocessing list with the same method including the same summary report.

It is highly recommended that the summary report name be defined directly in the method (summary report sub-section) rather than defining its name directly from the method properties screen in the sequence (or reprocessing list).

Suitability Tests - The sample type is taken into account for the suitability actions only that means a result is computed for each suitability test whatever the sample type is. This is a normal behavior.

Temporary Files - The *.DEC files can be deleted manually. One DEC file is created per sequence. The deletion has no impact on the normal use of the software. These files are normally stored in C:\WINNT or C:\TEMP. Use the Start/Find option to be sure to find all the *.DEC files.

Variables - The Deltat variable (1/acquisition rate) is displayed with 2 decimals in the chromatogram properties. Depending on the acquisition rate, 0.00 may be displayed. The workaround is to create a new global user formula variable (formula: = DELTAT) and to select more decimals to display.

The value of the Samplename variable is always N.A. A workaround is to use the Runname variable that corresponds to the chromatogram's name instead of this one.

It is not recommended to change the type of a user formula variable as results are not automatically updated after a reprocess (F6). The workaround is to reintegrate (F5) the chromatogram before reprocessing of the chromatogram.

Notes on CompassCDS Report Editor

Open File - Use the Open button to open a report style. Double-clicking on the file name may cause some coordinates to be changed.

Chromatogram - The default format for peak and group reports corresponds to the format defined in the chromatogram whereas the chromatogram default format corresponds to the software format.

Printing the Method - Peak user-input variables applied to data are not saved within the method, and therefore are not printed in the Chromatogram Method Report. The reference column is always printed as part of the peak identification table in the Chromatogram Method Report. If no reference peak is defined, the column will be printed with the header: 'Ref?', but left blank.

Text and Label - If defining $PAGENUM or $PAGECOUNT variables in a text or label object and that the variable name is cut in the report template (because the text /label object is not large enough), then the value of the variable is not printed in the report but $PAGENUM or $PAGECOUNT is printed. Enlarge the text or label object in the report template to solve the issue.

Notes on CompassCDS Configuration Manager

General - When the NexusDB Server service has been stopped for any reason, it should be manually restarted otherwise it will not be possible to log in the Configuration Manager.

The following limitations are present in the Configuration Manager compared to versions prior to 1.8:

Group, project, user, user profile, administrator profile, system and station names do not exceed 40 characters.

User initials do not exceed 4 characters.

Accents, parentheses, ‘, “, ^, ¨, or µ characters are forbidden in item names (group, project, user, profile, system and station). Parentheses are also forbidden in injector and detector names.

These limitations have been added to fix or prevent potential problems.

Configuration - After changing some parameters from the Configuration menu (security, electronic signature…. Parameters), it is recommended to exit CompassCDS and to login again instead of selecting the Session/New Login option.

By default, a Group1 is created, a default template path is defined in its properties: C:\CompassCDS\data\template, but the corresponding directory does not exist on the station. The workaround is to edit the group1 properties, and answer yes to the message prompting the user to create the template path.

Printing System Configuration - When you print the system configuration, an additional blank page is printed.

System - When renaming some channels, detectors are not sorted by alphabetical order in the system tree view. Moreover, when creating a system with several injectors and detectors, they are not sorted by alphabetical order before the database is refreshed (F5). When some drivers have been updated, the corresponding devices version may not be refreshed properly in the system properties. The workaround is to refresh the view (F5).

System Properties - When you change the system name or the signal unit in the configuration manager, you need to restart the CompassCDS session to update the acquisition window. Otherwise, the old name and unit will be displayed.

Users - Defining the same user several times with different profiles in a given group/project is not possible.

Plug-ins and Add-ons

Enhanced Chromatogram Report – New version replaces the Multi-Channel Chromatogram Report. Users can create customized reports as a single report for up to 4 channels, and peak and group results can be displayed separated by channel or combined into one single table each. Supports now also QTY normalization over up to 4 channels. Report can be executed in direct mode via the toolbar menu or during reprocessing of the chromatogram.

1-Button Interface - An easy-to-install simplified graphical user interface with a CompassCDS administrator accessible configuration screen that enables runs to be set up by operators using individual icons to specify the type and number of sample runs, multi-level calibrations, control sample and blank runs and, if required, continuous looping runs for routine samples taken from the continuous gas or liquid flow or storage tanks via valve injection. The new version also supports sample injection from controlled autosamplers, and entering of text that is displayed thereafter in the run info field of the chromatogram.

Currently the 1-Button interface can only be used with one CompassCDS Project per logon even though the All Projects mode can be selected.

Hydrocarbon Reporting Tool – Special plugin for the hydrocarbon processing industry focusing on ASTM, GPA and ISO based calculations for gases and liquids. Report and calculations can be flexibly setup and executed in direct mode or as a post-run process. Calculations include component, summary and extended calculations. Additionally, the Hydrocarbon Calculation Tool supports custom calculations and automated export of report details and calculated results in XML format.

CompassCDS AnIML Converter - Add-on for long-term archiving of chromatogram raw data, meta data and results in a human readable AnIML file format. AnIML file can be also used to extract and upload of chromatogram results into LIMS or SAP/ERP. Converter can be used in automatic mode as post-run executable file, or by drag & drop of chromatograms into the CompassCDS Viewer component.

CompassCDS AnIML Viewer – Viewer component for AnIML files. Allows to display and fully review and process chromatogram details (raw data, meta data and results) without compromise even after a long period of time and the need to have CompassCDS available on the computer.

CompassCDS
Installation Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501483
Revision E

Contents

Installation Prerequisites common to all CompassCDS installations 3
RAM Memory Requirements 3
Windows Services and Memory Utilization 3
CompassCDS Pre-installation Checklist 3

CompassCDS Standalone Workstation Software Installation Instructions 5
Preparing a Computer for CompassCDS Standalone Software Installation 5
Installing the CompassCDS Standalone Software on a suitably prepared Windows Computer 5

CompassCDS Server Core Software Installation Instructions 9
Preparing a Windows Server for CompassCDS Server Software Installation 9
Windows Server 2008 Software Installation Instructions 10
Windows Server 2012 R2 / 2016 Software Installation Instructions 11
Installing the CompassCDS Server Core Software on a prepared Windows Server 16
Uninstalling CompassCDS 19

CompassCDS Client Software Installation Instructions 21
Preparing a Windows Computer for CompassCDS Client Software Installation 21
Installing CompassCDS client Software on a suitably prepared Windows computer 21

CompassCDS DCOM and Folder Permission Setting Tool 25
CompassCDS Folder Access Permission Configuration 27
CompassCDS File Type Descriptions 29
Windows Services 31
Routine CompassCDS System Maintenance 31
Recommended backup and recovery procedure for CompassCDS Workstation and Main Server Installations 32

CompassCDS Troubleshooting Tips 34
Networking 34
CompassCDS Software Installation Qualification 34

CompassCDS Instrument Control Drivers 37
Principles 37
File Locations 37

Instruments Control Driver Installation 38
Scion Instruments 400 Series GC 38

BOOTP Server Configuration 40

System Configuration 43
Scion Instruments GC Systems 43
Checklist for CompassCDS Installation 47

Appendix 1 48
DCOM Configuration under Windows 2003 Server 48
DCOM Configuration Under Windows XP SP2, Windows 2003 58

Installation Prerequisites common to all CompassCDS installations

RAM Memory Requirements

Memory requirements of CompassCDS are listed below according to the Operating System.

Operating System	Minimum RAM (GB)	Recommended RAM (GB)	Virtual Memory (GB)
Windows 7 Professional/Ultimate/ Enterprise	4	8	4000
Windows 10 Pro/Enterprise	4	8	4000
Windows Server 2008 R2	8	16/32	4000
Windows Server 2012 R2	8	16/32	4000
Windows Server 2016	8	16/32	4000

Windows Services and Memory Utilization

The CompassCDS computer(s) should be a machine dedicated for purpose due to the limited number of Windows services that can be created on each computer as CompassCDS creates two new Windows services (Acquisition & Control System and Quick Start Engine) each time a system (instrument) is created.

CompassCDS Pre-installation Checklist

- ✓ All but one Network Interface Cards (usually the onboard NIC with static IP) must be temporarily disabled for the duration of the installation process. If additional Network Interface Cards (NICs) are present, (Wireless, VPN, VM), these must be disabled during the installation process. If this is not done during installation, users may observer a REG.C error when logging in to CompassCDS.
- ✓ The software installer must have Local Administrator level access during the installation in the case of standalone installations and Domain Administrator level access in the case of client/server or network installations (following network installs the default user level should be Domain User).
- ✓ Under Windows 7 and Windows Server 2008/2012, the property "Allow the computer to turn off this device to save power" is checked by default. This can cause serious communication issues with CompassCDS therefore all power management settings for all network (NIC) cards must be turned off.
- ✓ Windows Firewall (including Domain Firewall) must be turned off for duration of the installation.
- ✓ Any Anti-virus software must be temporarily disabled for duration of install and exclusions for certain CompassCDS folders should be set post install.

- ✓ Check that DEP (Data Execution Prevention) is de-activated for all except Microsoft Applications. To deactivate DEP, select: ‘System Properties\ Advanced\ Performance Settings\ Data Execution Prevention tab\’. Check the ‘Turn on DEP’ for essential Windows Programs and Services only option.
- ✓ It is recommended that all screen savers be disabled.
- ✓ CompassCDS requires that the display must be set to at least 1024 x 768 pixels and 16-bit color. To change these settings: right-click on the Windows Desktop and select Properties, Screen Resolution. Click on the Settings Tab to adjust screen resolution and color depth.
- ✓ It is recommended that the display font size be set to 96 DPI to correctly use CompassCDS. For Windows 7 installations, this setting can be found under Control Panel\Appearance and Personalization\Display\Set Custom Text Size (DPI)
- ✓ A formatted (NTFS) primary disk partition of at least 100 GB exists on the server onto which the CompassCDS server software is to be installed.

CompassCDS Standalone Workstation Software Installation Instructions

Preparing a Computer for CompassCDS Standalone Software Installation

The CompassCDS software should only be installed on one of the following Windows operating systems:

- Windows 7 Professional Service Pack 1 (32 or 64 bit)
- Windows 7 Enterprise Service Pack (32 or 64 bit)
- Windows 7 Ultimate Service pack 1 (32 or 64 bit)
- Windows 10 Pro (32 or 64 bit)
- Windows 10 Enterprise (32 or 64 bit)

If the CompassCDS software is being installed onto a computer that is part of an existing company or corporate local area network (LAN), ensure that the following checklist is completed before the CompassCDS software install begins.

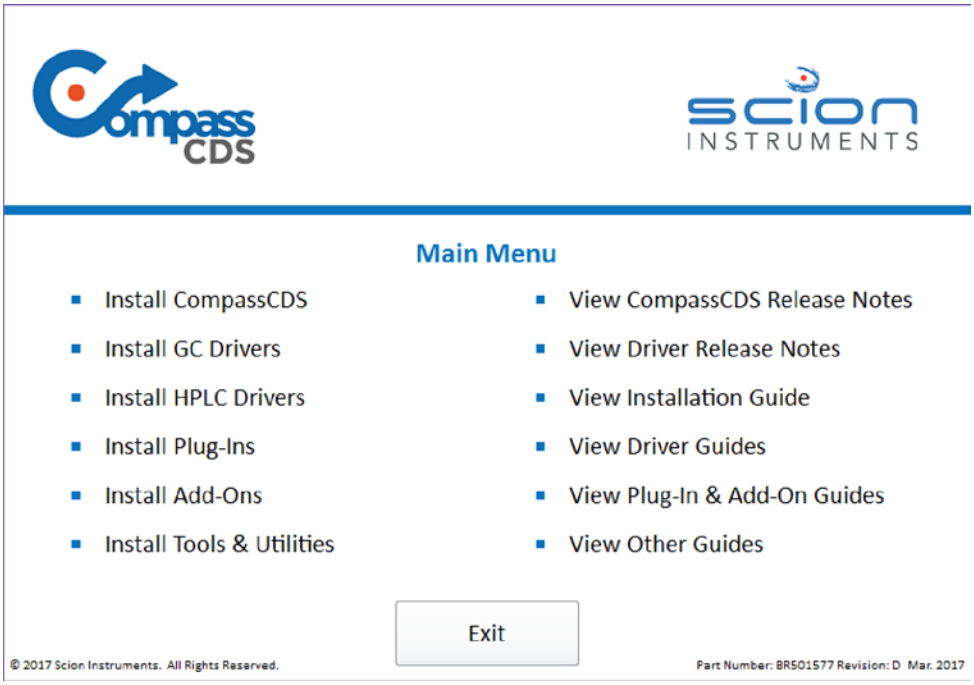
- ✓ The networked computer onto which the CompassCDS standalone software is to be installed has at least one static IP, a suitable subnet mask and, if required, a gateway IP.

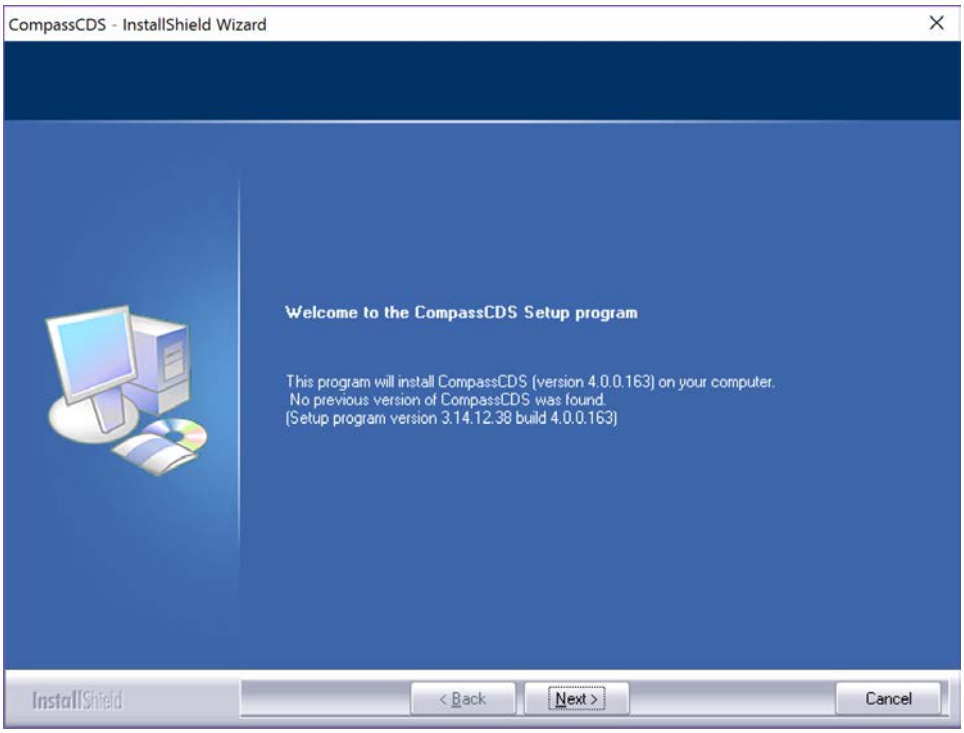
If the CompassCDS standalone software is being installed onto a new standalone computer that will not be part of a company local area network (LAN), ensure that the following computer related checklist is completed before the CompassCDS standalone software install begins.

- ✓ The computer onto which the CompassCDS standalone software is to be installed has at least one static IP, a suitable subnet mask (and if required, a gateway IP)

Installing the CompassCDS Standalone Software on a suitably prepared Windows Computer

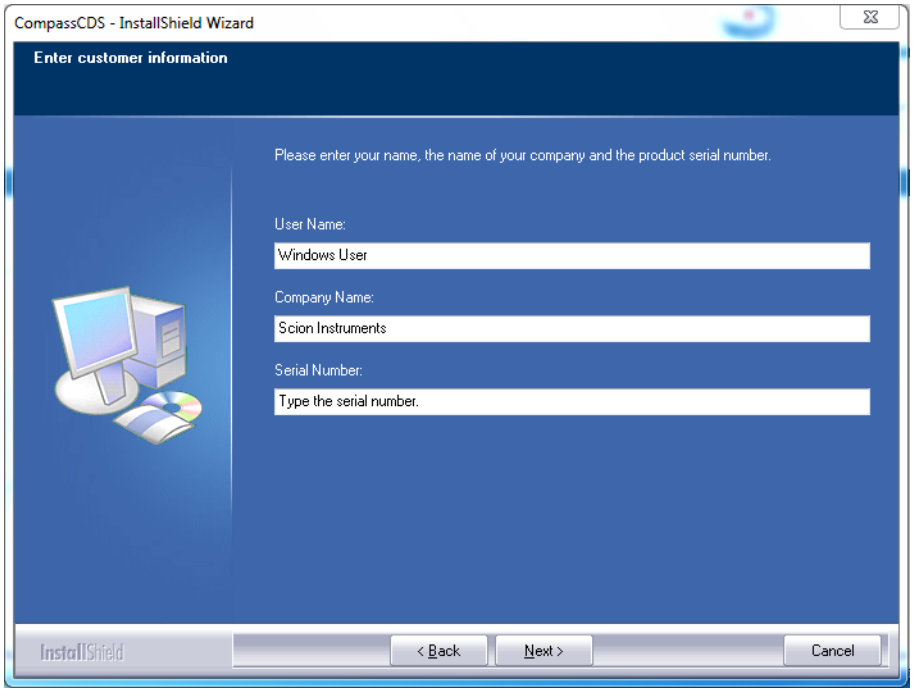
1. Refer to Appendix 1 for minimum recommended computer specifications
2. Ensure installer has local administrator rights for this computer.
3. If a legacy Galaxie installation exists, execute following steps:
    - Uninstall Galaxie via Windows Add Remove Programs
    - When requested, Reboot computer
    - After the reboot, go to C:\ Galaxie and copy the C:\Galaxie\Data folder to a different location.
    - Delete the C:\Galaxie folder and all subfolders
4. Insert the CompassCDS software media, and select the Install CompassCDS menu option (shown below). If the installation menu does not load, navigate to the CD/DVD drive (usually D:) and select the autorun option.




CompassCDS - InstallShield Wizard
Welcome to the CompassCDS Setup program
This program will install CompassCDS (version 4.0.0.163) on your computer.
No previous version of CompassCDS was found.
(Setup program version 3.14.12.38 build 4.0.0.163)
InstallShield
< Back
Next >
Cancel

5. Click Next, Next, Yes to accept the software license terms and then select the Standalone option and click Next.

6. Fill in the User Name, Company and CompassCDS Base License Serial Number provided as shown below.



7. Click Next, Next, Next and the CompassCDS software installation will proceed. When prompted, select the Restart Computer now option and the computer will initiate a re-boot sequence.

8. After the computer has completed re-booting, press Control + Alt + Delete keys and log on using the local administrator login.

9. The CompassCDS installation will continue and complete with the following message “Congratulations, you have successfully installed CompassCDS. Click Finish

10. Log into Compass Configuration Manager using:

    User: admin

    Password: compass

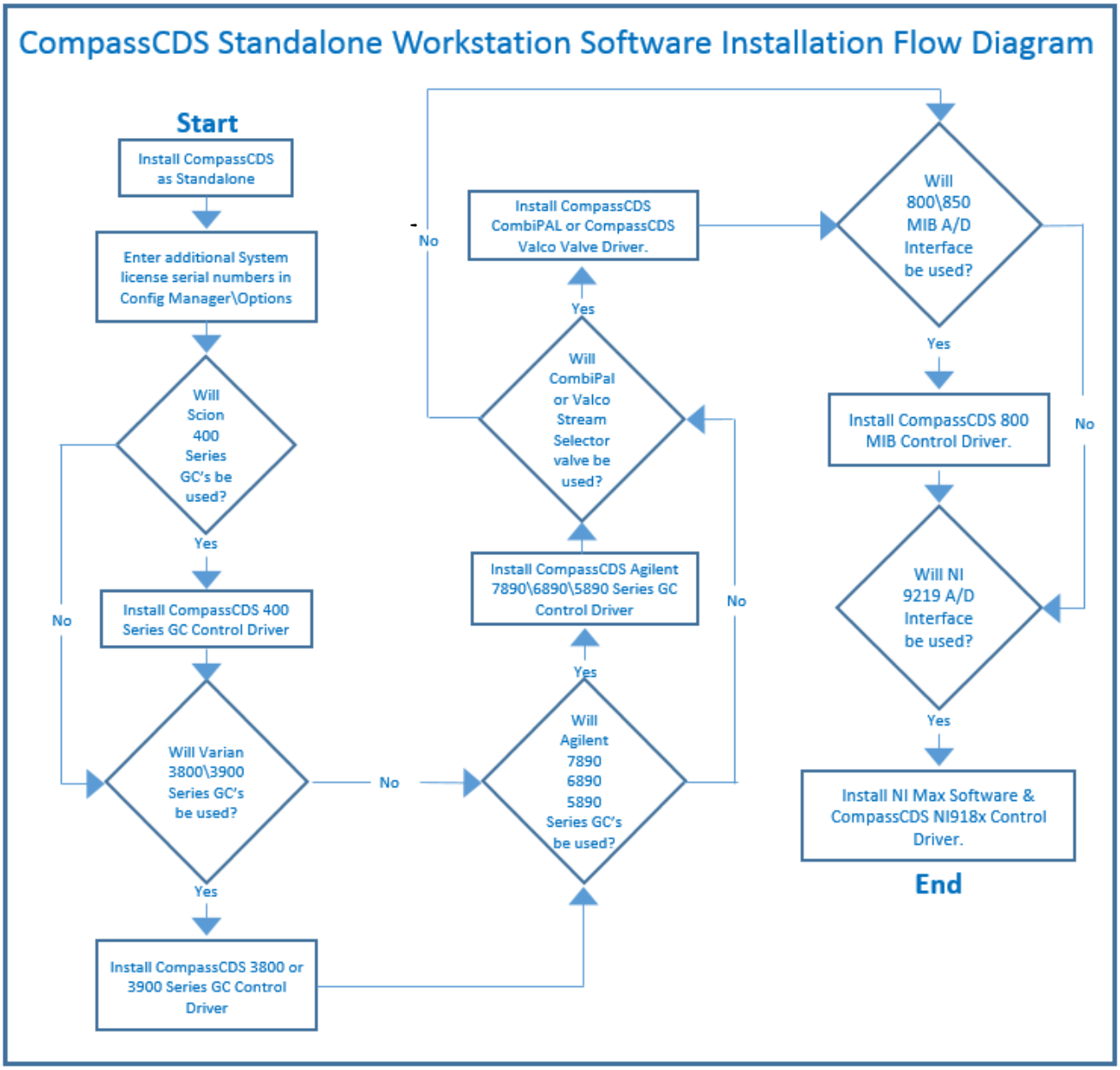
    Confirm from the top menu in Configuration Manager >Options> Licenses that the serial number entered during the initial part of the install process is listed.

11. Enter any additional System (instrument) license serial numbers by selecting the Options, Licenses, Add option.

12. CompassCDS instrument control drivers should now be installed on the CompassCDS server as this computer has automatically been designated as an acquisition & control server which means that it can “own” and control GC and LC instruments. A CompassCDS standalone software flow diagram (see below) indicates the way the instrument control drivers should be installed. To install the CompassCDS instrument control drivers, select the Drivers and Manuals menu option from the CompassCDS install CD and then select the appropriate driver set to install. Enter the appropriate serial number when prompted and let the installation complete.

13. The CompassCDS standalone software is now installed.

IMPORTANT NOTE: If any warning messages appear during the installation stating that "This service already exists….", continue with the installation and once complete, un-install CompassCDS and then re-install the software a second time. This will rectify this problem as the un-install procedure will successfully remove these services. The service(s) being referred to in the error/warning messages are artifacts from an incomplete un-install of either Galaxie or an earlier version of CompassCDS and if these are not removed, these services (usually acquisition and control) will appear to be present but will be non-functional.


CompassCDS Standalone Workstation Software Installation Flow Diagram
Start
Install CompassCDS as Standalone
Enter additional System license serial numbers in Config Manager\Options
Will Scion 400 Series GC's be used?
Yes
No
Install CompassCDS 400 Series GC Control Driver
Will Varian 3800\3900 Series GC's be used?
Yes
No
Install CompassCDS 3800 or 3900 Series GC Control Driver
Will Agilent 7890 6890 5890 Series GC's be used?
Yes
No
Install CompassCDS Agilent 7890\6890\5890 Series GC Control Driver
Will CombiPal or Valco Stream Selector valve be used?
Yes
No
Install CompassCDS CombiPAL or CompassCDS Valco Valve Driver.
Will 800\850 MIB A/D Interface be used?
Yes
No
Install CompassCDS 800 MIB Control Driver.
Will NI 9219 A/D Interface be used?
Yes
Install NI Max Software & CompassCDS NI918x Control Driver.
End

CompassCDS Server Core Software Installation Instructions

Preparing a Windows Server for CompassCDS Server Software Installation

The CompassCDS server core software should only be installed on one of the following Windows Server operating systems:

- Windows Server 2008 R2 Standard 32 or 64 bit (Full Installation)
- Windows Server 2008 R2 Enterprise 32 or 64 bit (Full Installation)
- Windows Server 2008 R2 Data Center 32 or 64 bit (Full Installation)
- Windows Server 2012 R2 64 bit (Full Installation)
- Windows Server 2016 64 bit (Full Installation)

If the CompassCDS server core software is being installed onto a server that is part of an existing company or corporate local area network (LAN), ensure that the following network/server related checklist is completed before the CompassCDS server software install begins.

- ✓ The server onto which the CompassCDS server core software is to be installed is a member of a Windows Domain with Windows Active Directory and DNS services active on this domain.
- ✓ This server should also have the server role of File Server.
- ✓ The Server onto which the CompassCDS server core software is to be installed has at least one static IP, a suitable subnet mask (and if required, a gateway IP) and an assigned DNS server address.
- ✓ The software installer has Domain Administrator level access during the installation (following install default user level should be Domain User).

If the CompassCDS server core software is being installed onto a brand-new server that will not be part of a corporate network, ensure that the following network/server related checklist is completed before the CompassCDS server core software install begins.

- ✓ The server onto which the CompassCDS server core software is to be installed as a Primary Domain Controller (PDC) with Windows Active Directory and DNS services active for the domain (usually designated as *DOMAINNAME*.*LOCAL*. Step-by-step Windows Server 2008 software installation instructions are described directly below this checklist.
- ✓ Additional server roles that should be installed on this server should include File Server and DHCP server with a defined IP scope.
- ✓ The Server onto which the CompassCDS server core software is to be installed has at least one static IP, a suitable subnet mask (and if required, a gateway IP) and an assigned DNS server address.
- ✓ The software installer has Domain Administrator level access during the installation (following install default user level should be Domain User).

Windows Server 2008 Software Installation Instructions

1. Insert Windows Server installation media
2. When prompted, select the Windows Server 2008 R2 version required for the install
    - Windows Server 2008 R2 Standard (Full Installation)
    - Windows Server 2008 R2 Enterprise (Full Installation)
    - Windows Server 2008 R2 Data Center (Full Installation)
3. Accept License Terms and select the custom install option (new copy of windows)
4. Select the correct primary disk partition and proceed with software installation.
5. Create a password suitable for Windows Server (alphanumeric with 1 upper case and 1 non-alphabetic) when prompted e.g., Compass1 Default server local login will be:

    User: Administrator

    PW: Compass1

6. When the installation has completed, the Windows Server Initial Configuration task window will appear. Perform the following tasks:
    - Activate Windows
    - Set time Zone
    - Configure NIC cards with static IPs, Subnet, Gateway and DNS (if not already done)
    - Disable NIC power management (if not already done)
    - Change computer name if required, e.g., Compass_server or as company required
    - Restart computer
7. Add server roles – click on server management icon on toolbar, select roles, add rolls
    - Active Directory domain services with Windows.Netframework 3.5.1
    - Add DHCP Server with defined IP scope
    - Add File Services
    - Promote the Server to a Domain Controller by running the dcpromo.exe (Start, Run, dcpromo.exe) and during this process, add a Domain Name (e.g. COMPASS.LOCAL)
8. This server should now be ready for the installation of the CompassCDS server software. Default server Domain login will be:

    User: COMPASS\Administrator

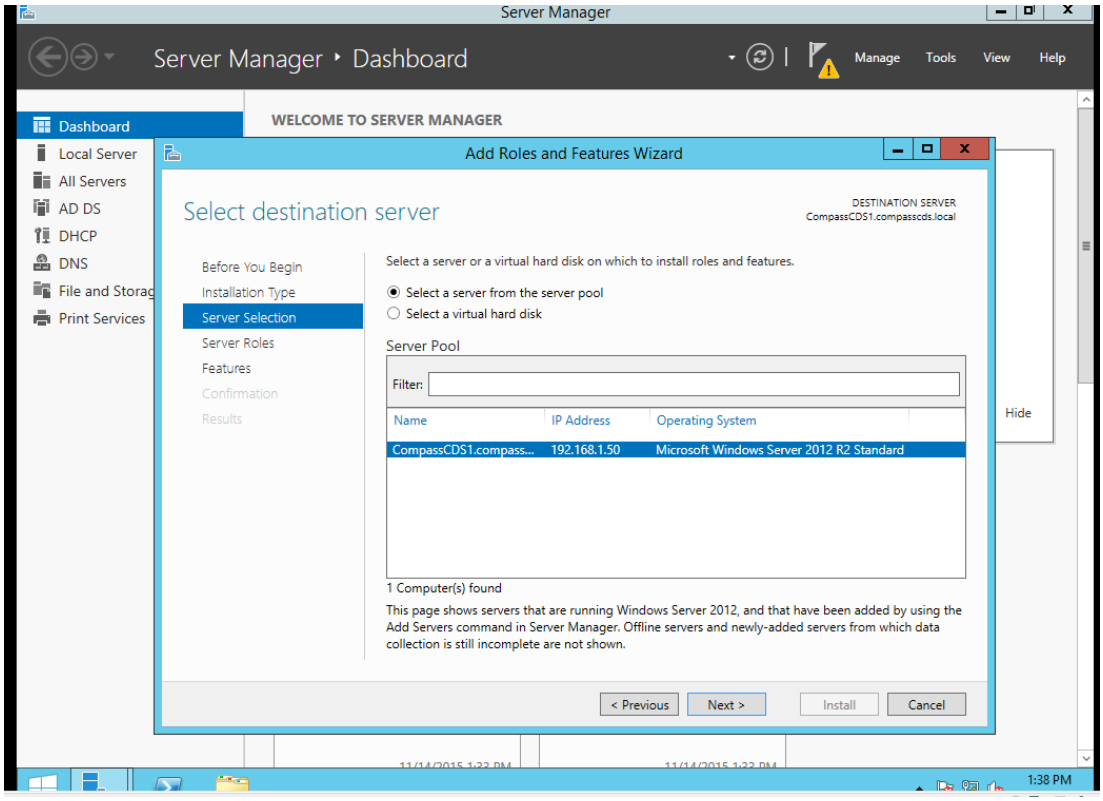
    Password: Compass1

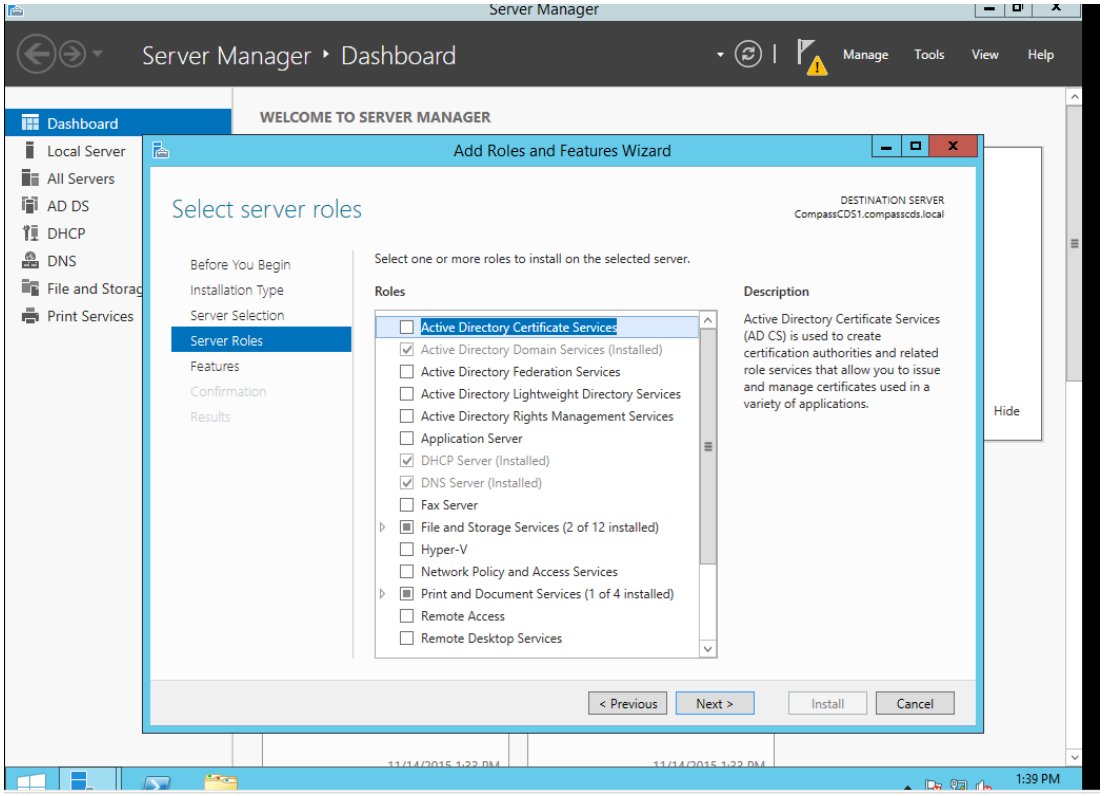
Windows Server 2012 R2 / 2016 Software Installation Instructions

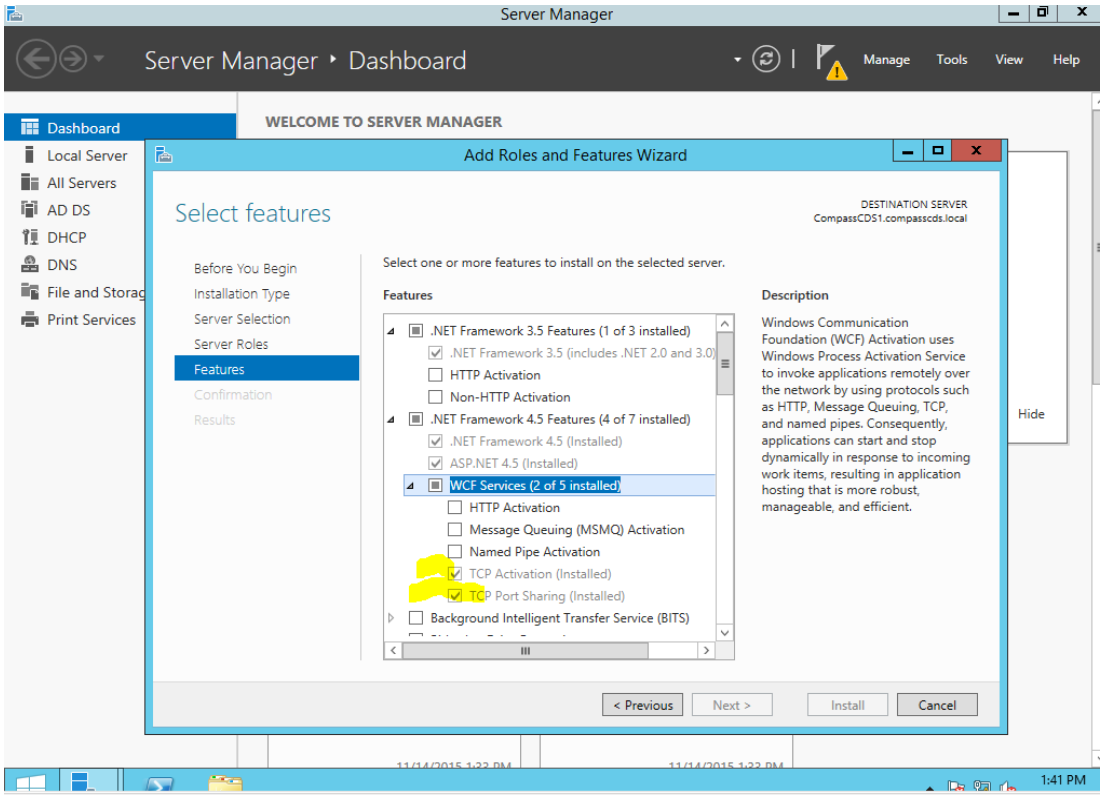
For a server that has already been prepared and is part of a company domain, contact the IT department to resolve the IP settings and the joining of the “domain”.

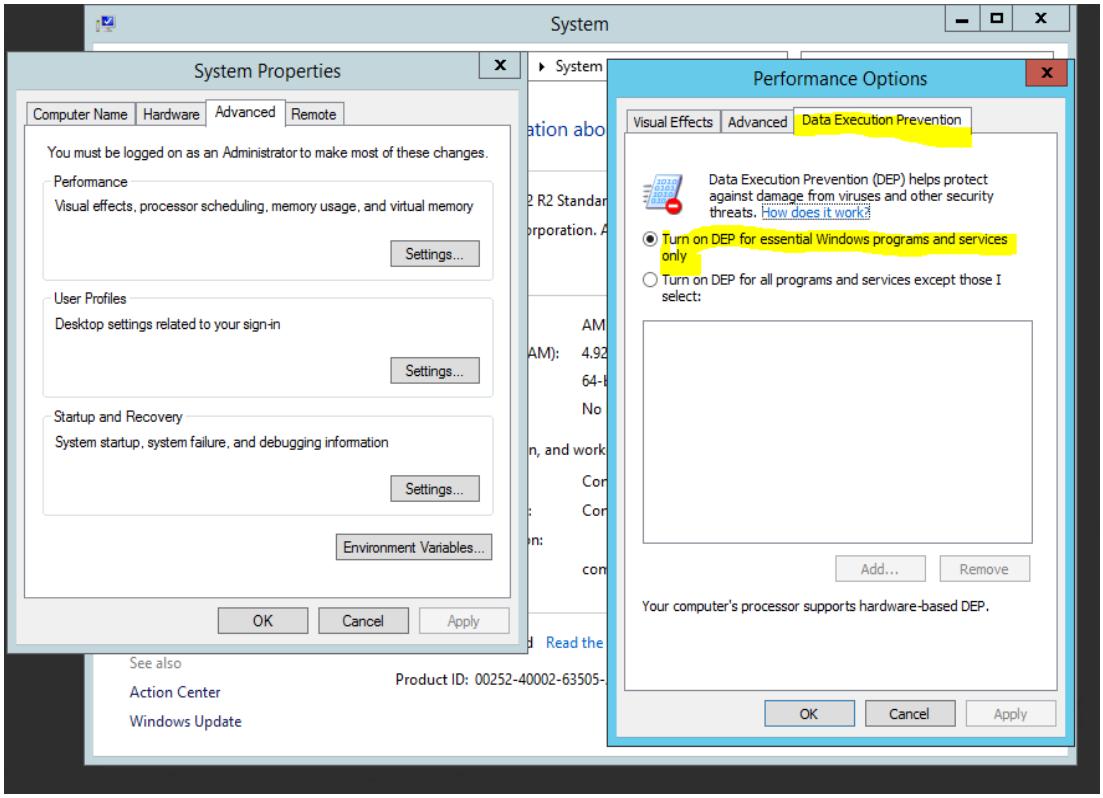
- One will still need a File server and print server role
- TCPIP will already be activated
- DEP must still be activated for Windows applications only
- Power management of the NIC’s will still need to be disabled (OFF)
- Windows Firewall still needs to be disabled
- Any anti-virus application cannot scan active CompassCDS directories
- When installing 2012R2 or 2016, follow the screenshots below to successfully implement the Operating System for preparation of a CompassCDS client server install. Starting at the Server Manager Dashboard continue with the steps listed below. This will prepare a private domain for your installation.

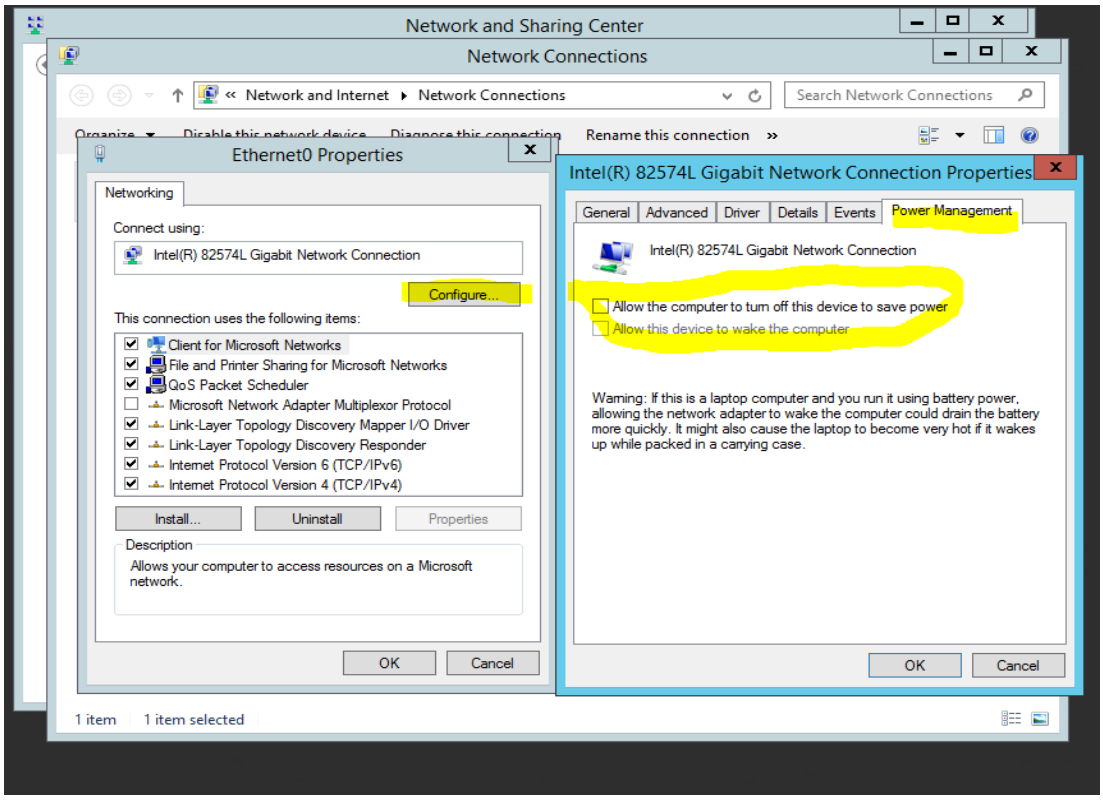
Only when you have been asked to create a private domain will you follow the following steps explicitly below.

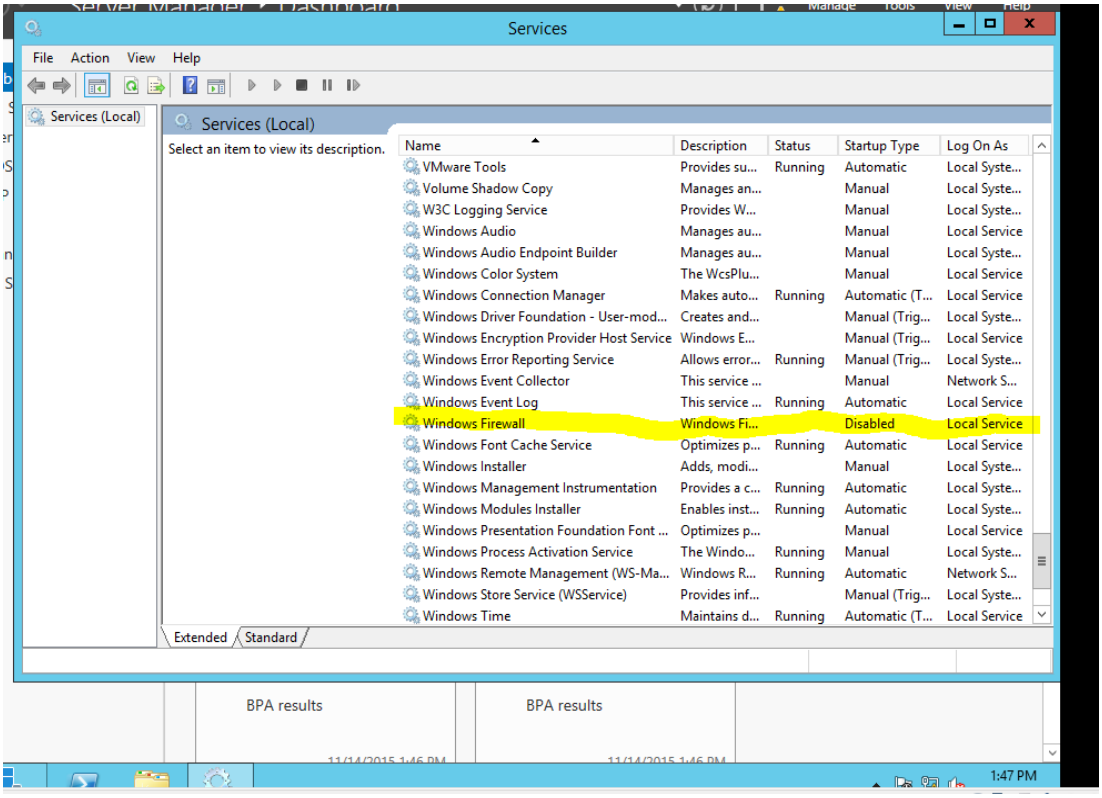


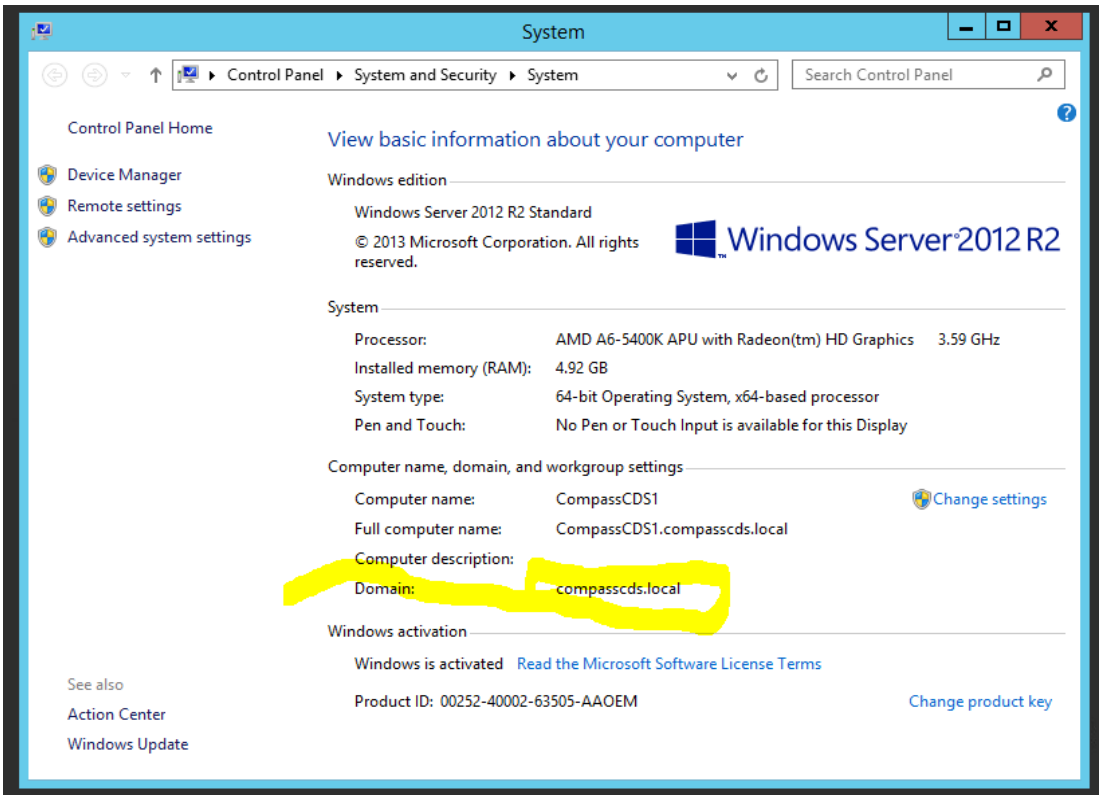

Server Manager
Server Manager ‣ Dashboard
Manage Tools View Help
Dashboard
Local Server
All Servers
AD DS
DHCP
DNS
File and Storag
Print Services
WELCOME TO SERVER MANAGER
Add Roles and Features Wizard
Select server roles
DESTINATION SERVER
CompassCDS1.compasscds.local
Before You Begin
Installation Type
Server Selection
Server Roles
Features
Confirmation
Results
Select one or more roles to install on the selected server.
Roles
Active Directory Certificate Services
Active Directory Domain Services (Installed)
Active Directory Federation Services
Active Directory Lightweight Directory Services
Active Directory Rights Management Services
Application Server
DHCP Server (Installed)
DNS Server (Installed)
Fax Server
File and Storage Services (2 of 12 installed)
Hyper-V
Network Policy and Access Services
Print and Document Services (1 of 4 installed)
Remote Access
Remote Desktop Services
Description
Active Directory Certificate Services (AD CS) is used to create certification authorities and related role services that allow you to issue and manage certificates used in a variety of applications.
< Previous
Next >
Install
Cancel
Hide
1:39 PM

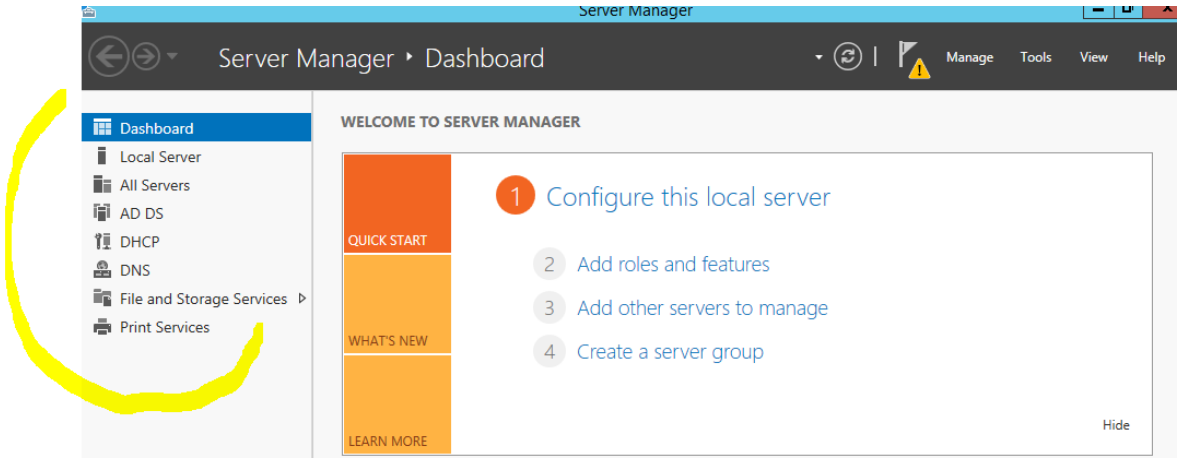

Server Manager
Server Manager ‣ Dashboard
Manage Tools View Help
Dashboard
Local Server
All Servers
AD DS
DHCP
DNS
File and Storag
Print Services
WELCOME TO SERVER MANAGER
Add Roles and Features Wizard
Select features
DESTINATION SERVER
CompassCDS1.compasscds.local
Before You Begin
Installation Type
Server Selection
Server Roles
Features
Confirmation
Results
Select one or more features to install on the selected server.
Features
.NET Framework 3.5 Features (1 of 3 installed)
.NET Framework 3.5 (includes .NET 2.0 and 3.0)
HTTP Activation
Non-HTTP Activation
.NET Framework 4.5 Features (4 of 7 installed)
.NET Framework 4.5 (Installed)
ASP.NET 4.5 (Installed)
WCF Services (2 of 5 installed)
HTTP Activation
Message Queuing (MSMQ) Activation
Named Pipe Activation
TCP Activation (Installed)
TCP Port Sharing (Installed)
Background Intelligent Transfer Service (BITS)
Description
Windows Communication Foundation (WCF) Activation uses Windows Process Activation Service to invoke applications remotely over the network by using protocols such as HTTP, Message Queuing, TCP, and named pipes. Consequently, applications can start and stop dynamically in response to incoming work items, resulting in application hosting that is more robust, manageable, and efficient.
< Previous
Next >
Install
Cancel
Hide
1:41 PM

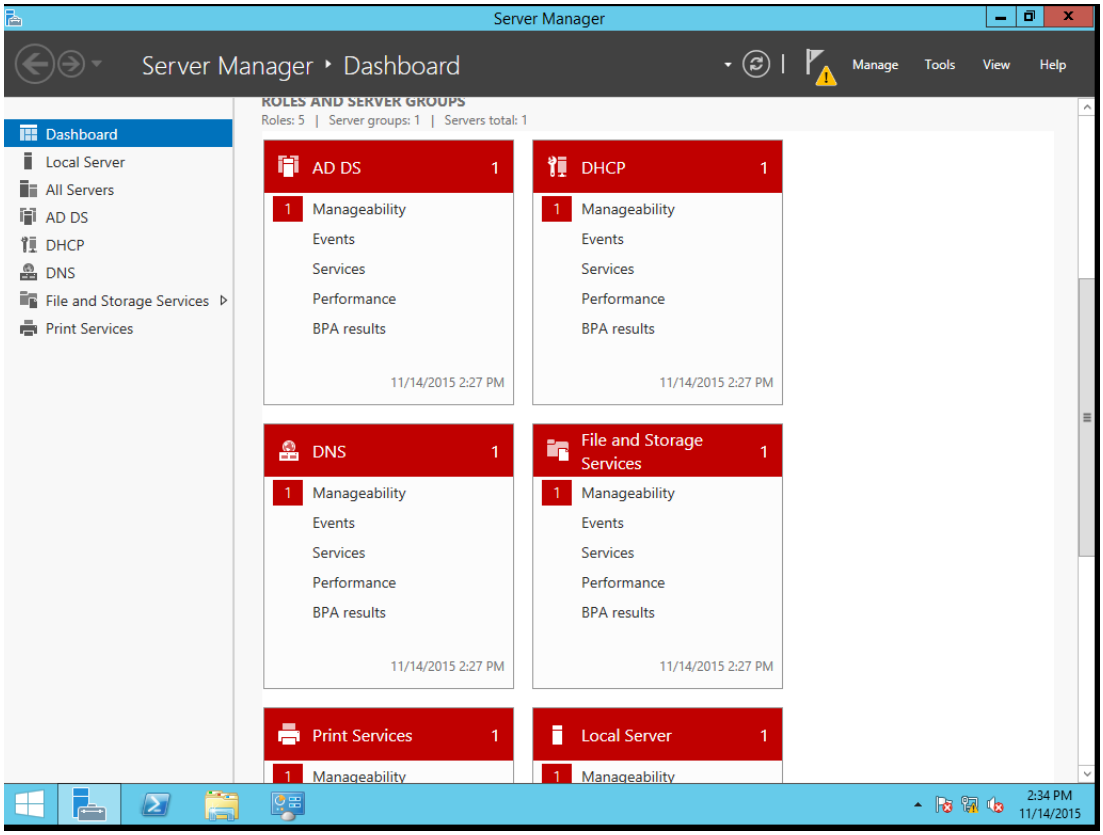

System
System Properties
Computer Name
Hardware
Advanced
Remote
You must be logged on as an Administrator to make most of these changes.
Performance
Visual effects, processor scheduling, memory usage, and virtual memory
Settings...
User Profiles
Desktop settings related to your sign-in
Settings...
Startup and Recovery
System startup, system failure, and debugging information
Settings...
Environment Variables...
OK
Cancel
Apply
See also
Action Center
Windows Update
Performance Options
Visual Effects
Advanced
Data Execution Prevention
Data Execution Prevention (DEP) helps protect against damage from viruses and other security threats. How does it work?
Turn on DEP for essential Windows programs and services only
Turn on DEP for all programs and services except those I select:
Add...
Remove
Your computer's processor supports hardware-based DEP.
OK
Cancel
Apply


Network and Sharing Center
Network Connections
Network and Internet
Network Connections
Search Network Connections
Rename this connection
Ethernet0 Properties
Networking
Connect using:
Intel(R) 82574L Gigabit Network Connection
Configure...
This connection uses the following items:
Client for Microsoft Networks
File and Printer Sharing for Microsoft Networks
QoS Packet Scheduler
Microsoft Network Adapter Multiplexor Protocol
Link-Layer Topology Discovery Mapper I/O Driver
Link-Layer Topology Discovery Responder
Internet Protocol Version 6 (TCP/IPv6)
Internet Protocol Version 4 (TCP/IPv4)
Install...
Uninstall
Properties
Description
Allows your computer to access resources on a Microsoft network.
OK
Cancel
Intel(R) 82574L Gigabit Network Connection Properties
General
Advanced
Driver
Details
Events
Power Management
Intel(R) 82574L Gigabit Network Connection
Allow the computer to turn off this device to save power
Allow this device to wake the computer
Warning: If this is a laptop computer and you run it using battery power, allowing the network adapter to wake the computer could drain the battery more quickly. It might also cause the laptop to become very hot if it wakes up while packed in a carrying case.
OK
Cancel
1 item
1 item selected


Services
File Action View Help
Services (Local)
Services (Local)
Select an item to view its description.
Name Description Status Startup Type Log On As
VMware Tools Provides su... Running Automatic Local Syste...
Volume Shadow Copy Manages an... Manual Local Syste...
W3C Logging Service Provides W... Manual Local Syste...
Windows Audio Manages au... Manual Local Service
Windows Audio Endpoint Builder Manages au... Manual Local Syste...
Windows Color System The WcsPlu... Manual Local Service
Windows Connection Manager Makes auto... Running Automatic (T... Local Service
Windows Driver Foundation - User-mod... Creates and... Manual (Trig... Local Syste...
Windows Encryption Provider Host Service Windows E... Manual (Trig... Local Service
Windows Error Reporting Service Allows error... Running Manual (Trig... Local Syste...
Windows Event Collector This service ... Manual Network S...
Windows Event Log This service ... Running Automatic Local Service
Windows Firewall Windows Fi... Disabled Local Service
Windows Font Cache Service Optimizes p... Running Automatic Local Service
Windows Installer Adds, modi... Manual Local Syste...
Windows Management Instrumentation Provides a c... Running Automatic Local Syste...
Windows Modules Installer Enables inst... Running Automatic Local Syste...
Windows Presentation Foundation Font ... Optimizes p... Manual Local Service
Windows Process Activation Service The Windo... Running Manual Local Syste...
Windows Remote Management (WS-Ma... Windows R... Running Automatic Network S...
Windows Store Service (WSService) Provides inf... Manual (Trig... Local Syste...
Windows Time Maintains d... Running Automatic (T... Local Service
Extended Standard
BPA results
BPA results
1:47 PM


System
Control Panel ▸ System and Security ▸ System
Search Control Panel
Control Panel Home
Device Manager
Remote settings
Advanced system settings
View basic information about your computer
Windows edition
Windows Server 2012 R2 Standard
© 2013 Microsoft Corporation. All rights reserved.
Windows Server 2012 R2
System
Processor: AMD A6-5400K APU with Radeon(tm) HD Graphics 3.59 GHz
Installed memory (RAM): 4.92 GB
System type: 64-bit Operating System, x64-based processor
Pen and Touch: No Pen or Touch Input is available for this Display
Computer name, domain, and workgroup settings
Computer name: CompassCDS1
Change settings
Full computer name: CompassCDS1.compasscds.local
Computer description:
Domain: compasscds.local
Windows activation
Windows is activated Read the Microsoft Software License Terms
Product ID: 00252-40002-63505-AAOEM
Change product key
See also
Action Center
Windows Update



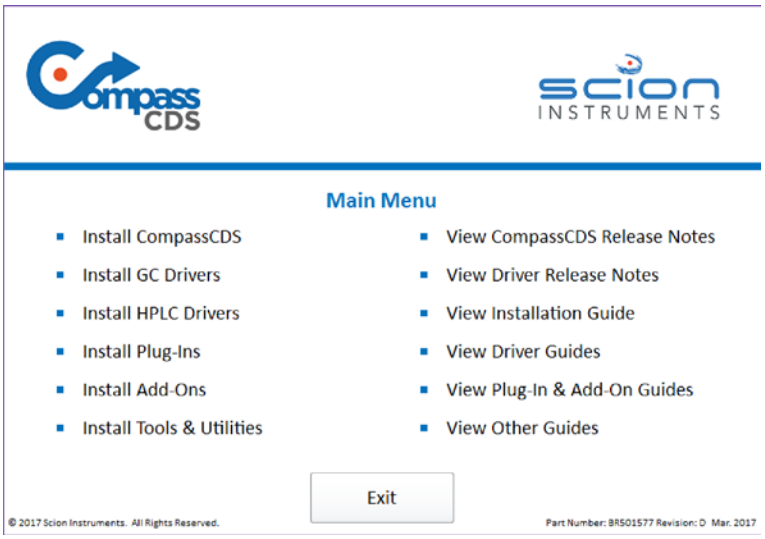


You must ignore the above errors in Server OS 2012R2/2016, close server manager and continue.

Next step is to install CompassCDS as a Main Server.

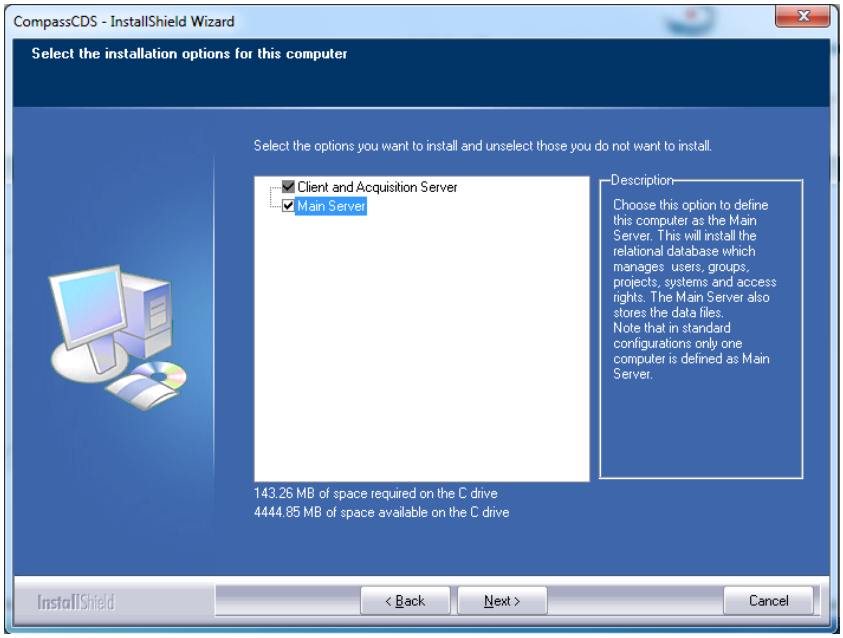
Installing the CompassCDS Server Core Software on a prepared Windows Server

1. Insert the CompassCDS software media, and select the Install CompassCDS menu option (shown below). If the installation menu does not load, navigate to the CD/DVD drive (usually D:) and select the autorun option.

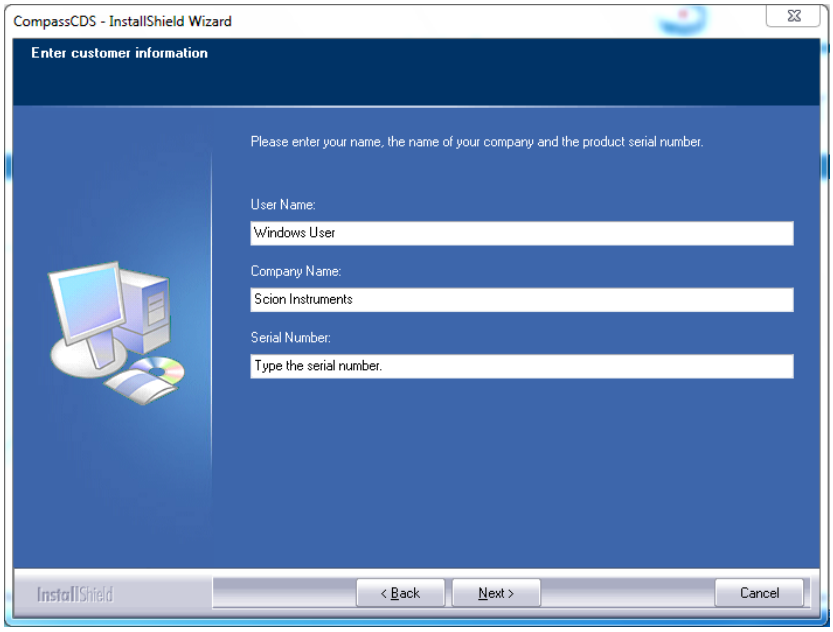


2. Click Next, Next, Yes to accept the software license terms and then select the Client/Server option and click Next. The Standalone install option is only used for non-client server CompassCDS installations as described in the preceding section.

3. Check the Client and Acquisition Server and Main Server option checkboxes (as shown below) and click Next.


CompassCDS - InstallShield Wizard
Select the installation options for this computer
Select the options you want to install and unselect those you do not want to install.
Client and Acquisition Server
Main Server
Description
Choose this option to define this computer as the Main Server. This will install the relational database which manages users, groups, projects, systems and access rights. The Main Server also stores the data files. Note that in standard configurations only one computer is defined as Main Server.
143.26 MB of space required on the C drive
4444.85 MB of space available on the C drive
InstallShield
< Back
Next >
Cancel

4. Fill in the User Name, Company and enter the CompassCDS Base License Serial Number provided as shown below.



5. Click Next, Next, Next and the CompassCDS software installation will proceed. When prompted, select the restart computer now option and the server will initiate a reboot sequence.

6. After the server has completed re-booting, press Control + Alt + Delete and log on to the Domain using the administrator login. A typical Windows domain logon using the COMPASS.LOCAL domain created earlier would be as follows:

   User: COMPASS\Administrator
   Password: Compass1

7. The CompassCDS installation will continue and complete with the following message “Congratulations, you have successfully installed CompassCDS. Click Finish

8. Log into Compass Configuration Manager using:

   User: admin
   Password: compass

   Confirm from the menu in Configuration Manager, Options, Licenses, which the serial number entered during the initial part of the install process is listed and reflects the correct number of System and Station licenses.

9. Enter any additional Station (computer) and System (instrument) license serial numbers by selecting the Add option.

10. CompassCDS instrument control drivers should now be installed on the CompassCDS server as this computer has been designated as an acquisition & control server which means that it can “own” and control GC and LC instruments. A CompassCDS server core software flow diagram (see below) indicates the way the instrument control drivers should be installed. To install the CompassCDS instrument control drivers, select the Drivers and Manuals menu option from the CompassCDS install CD and then select the appropriate

driver set to install. Enter the appropriate serial number when prompted and let the installation complete.

11. Check that Internet Explorer Active Scripting is enabled (Go to Internet Explorer, Tools, Internet Options, Security, Internet, Custom Level, Active Scripting – Enable).

12. Once the driver software installation has completed, select the Tools and Documentation option from the CompassCDS media and run the CompassCDS Diagnostics Tool. This tool will install an UltiPro web server as part of the CompassCDS Diagnostics Tool setup.

13. Run the CompassCDS DCOM Tool from the desktop icon and click on the CompassCDS Installation Analysis option. Click on Go and Fix Issues. Check that any flagged items (red) are now green. Close this window.

14. The CompassCDS server core software is now installed.

IMPORTANT NOTE: If any warning messages appear during the installation stating that "This service already exists….", continue with the installation and once complete, un-install CompassCDS and then re-install the software a second time. This will rectify this problem as the un-install procedure will successfully remove these services. The service(s) being referred to in the error/warning messages are artifacts from an incomplete un-install of either Galaxie or an earlier version of CompassCDS and if these are not completely removed, these services (usually acquisition & control) will appear to be present but will be non-functional.

NOTES: It is important to install and run the CompassCDS Diagnostics Tool after installing CompassCDS as a main server or client to automatically set all the required DCOM permissions correctly.

If error messages such as "Error extracting support files", "Error installing Ikernel .exe", "Access is denied", "Error loading type library/DLL" are displayed during the installation, it will be necessary to edit the registry as follows and then perform an uninstall and re-install of the CompassCDS software.

CAUTION Use caution when editing – edits to registry may severely damage your system.

15. Click on the 'Windows Start' button and select 'RUN'. Type REGEDIT and click 'OK'. In REGEDIT find and remove the key {2565438A-1759-4F9D-A14A-DB5BD0A22EB4} in:Hkey_local_machine \ Software\Microsoft \ Windows\CurrentVersion\Uninstall

16. Next remove the folder {2565438A-1759-4F9D-A14A-DB5BD0A22EB4} located in: 'Program Files \ InstallShield\ Installation Information'.

17. Then remove the contents of the folder where CompassCDS was installed, except for files with an extension: .DDB, .DDC and the generated files (DATA, .METH, .CALB.etc).

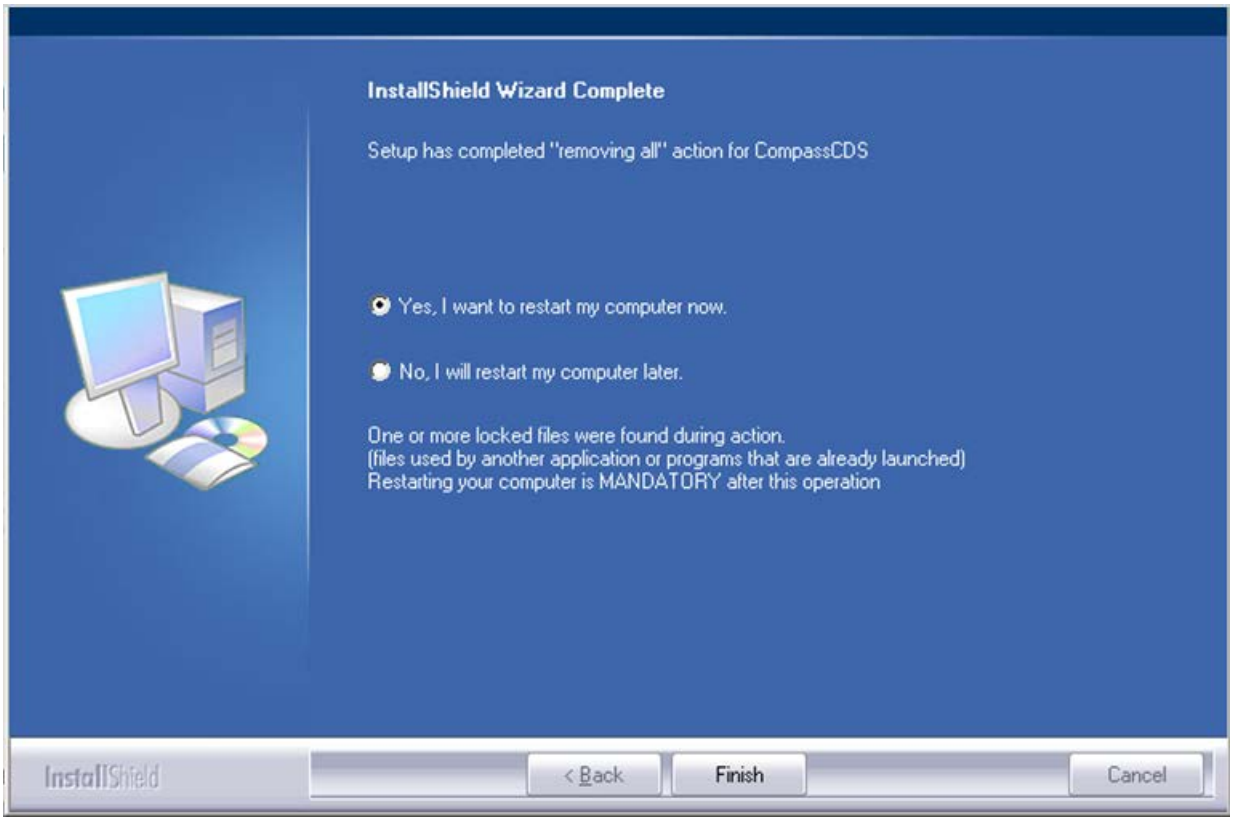
Uninstalling CompassCDS

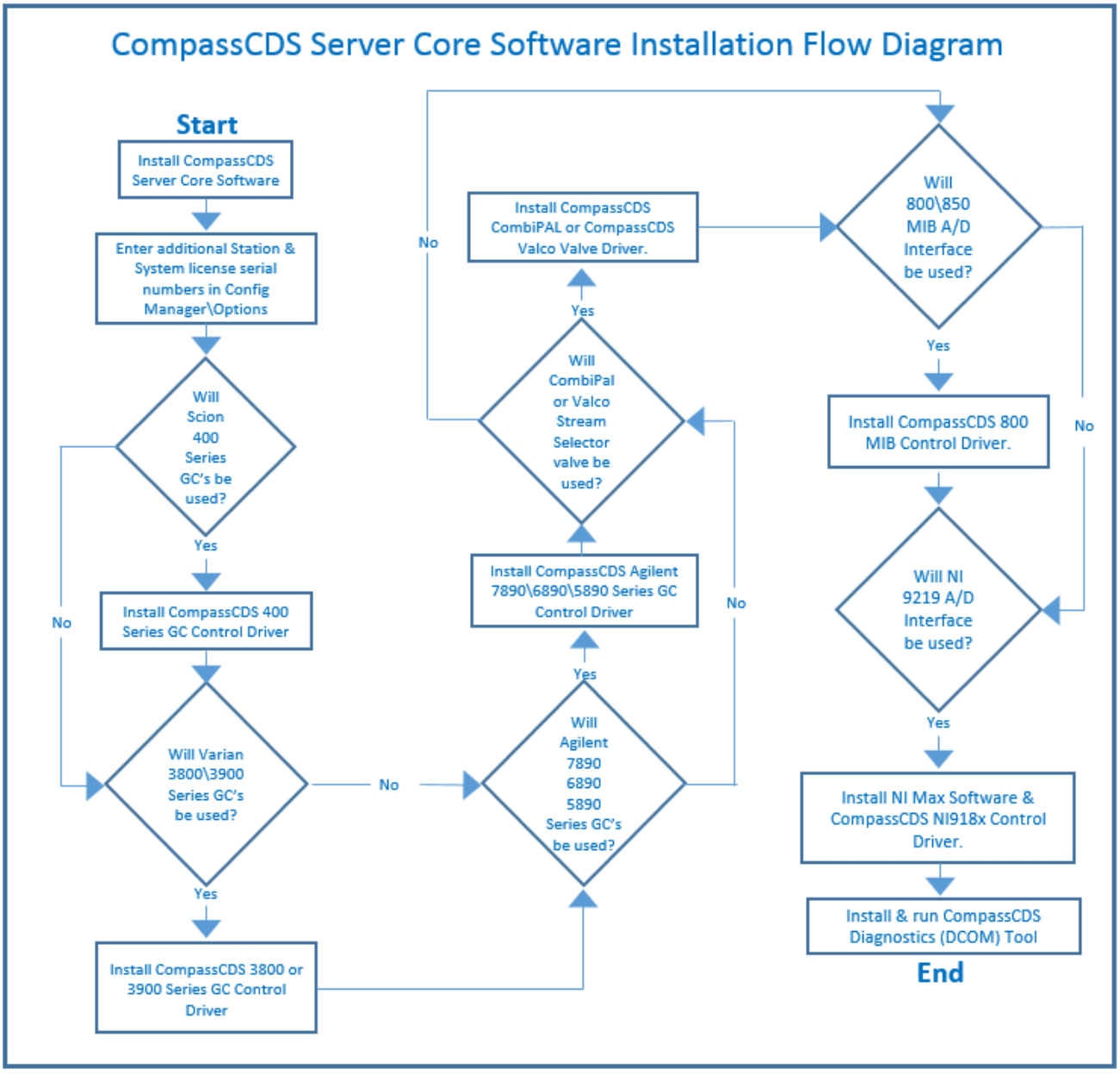
During the uninstall process, the following message asks the user to confirm the removal of the CompassCDS software. Click on ‘Yes’ to uninstall or ‘No’ to stop the uninstall process.

After all the files have been removed, the following dialog is displayed. Click on ‘Finish’.

A dialog box then appears indicating that the computer needs to be rebooted.

Click on ‘Finish’ to complete the software removal and reboot the computer.


InstallShield Wizard Complete
Setup has completed "removing all" action for CompassCDS
Yes, I want to restart my computer now.
No, I will restart my computer later.
One or more locked files were found during action.
(files used by another application or programs that are already launched)
Restarting your computer is MANDATORY after this operation
InstallShield
< Back
Finish
Cancel


CompassCDS Server Core Software Installation Flow Diagram
Start
Install CompassCDS Server Core Software
Enter additional Station & System license serial numbers in Config Manager\Options
Will Scion 400 Series GC's be used?
Yes
No
Install CompassCDS 400 Series GC Control Driver
Will Varian 3800\3900 Series GC's be used?
Yes
No
Install CompassCDS 3800 or 3900 Series GC Control Driver
Will Agilent 7890 6890 5890 Series GC's be used?
Yes
No
Install CompassCDS Agilent 7890\6890\5890 Series GC Control Driver
Will CombiPal or Valco Stream Selector valve be used?
Yes
No
Install CompassCDS CombiPAL or CompassCDS Valco Valve Driver.
Will 800\850 MIB A/D Interface be used?
Yes
No
Install CompassCDS 800 MIB Control Driver.
Will NI 9219 A/D Interface be used?
Yes
Install NI Max Software & CompassCDS NI918x Control Driver.
Install & run CompassCDS Diagnostics (DCOM) Tool
End

CompassCDS Client Software Installation Instructions

Preparing a Windows Computer for CompassCDS Client Software Installation

The CompassCDS client software should only be installed on one of the following Windows operating systems:

- Windows 7 Professional Service Pack 1 (32 or 64 bit)
- Windows 7 Enterprise Service Pack (32 or 64 bit)
- Windows 7 Ultimate Service Pack 1 (32 or 64 bit)
- Windows 10 Pro (32 or 64 bit)
- Windows 10 Enterprise (32 or 64 bit)

If the CompassCDS client software is being installed onto a computer that is part of an existing company or corporate local area network (LAN), ensure that the following network/server related checklist is completed before the CompassCDS client software install begins.

The computer onto which the CompassCDS server core software is to be installed is already a member of the same Windows Domain (with Windows Active Directory and DNS services active) onto which the CompassCDS server software was installed.

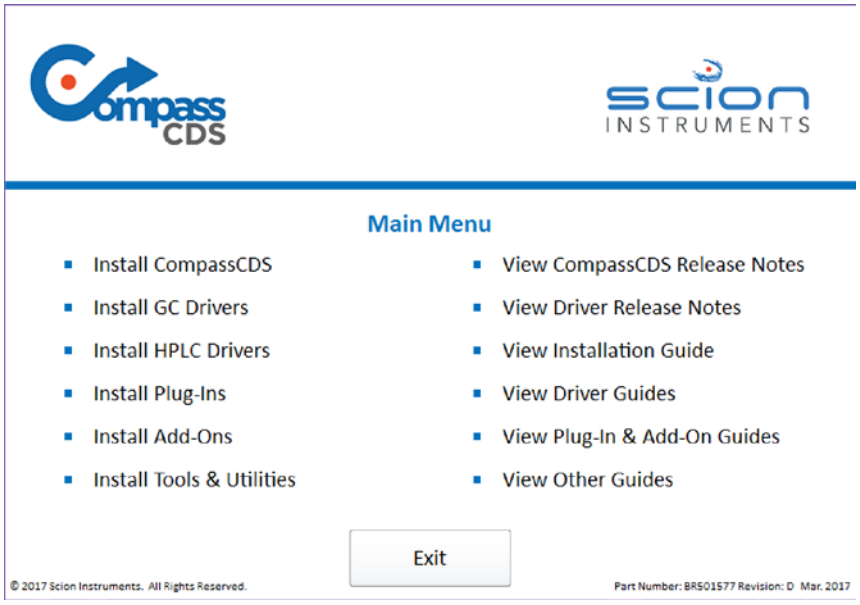
The computer onto which the CompassCDS server core software is to be installed has at least one static IP (if to be assigned as a CompassCDS acquisition and control server,) a suitable subnet mask (and if required, a gateway IP) and an assigned DNS server address, otherwise DHCP IP assignment will be adequate.

The software installer has Domain Administrator level access during the installation (following install default user level should be Domain User).

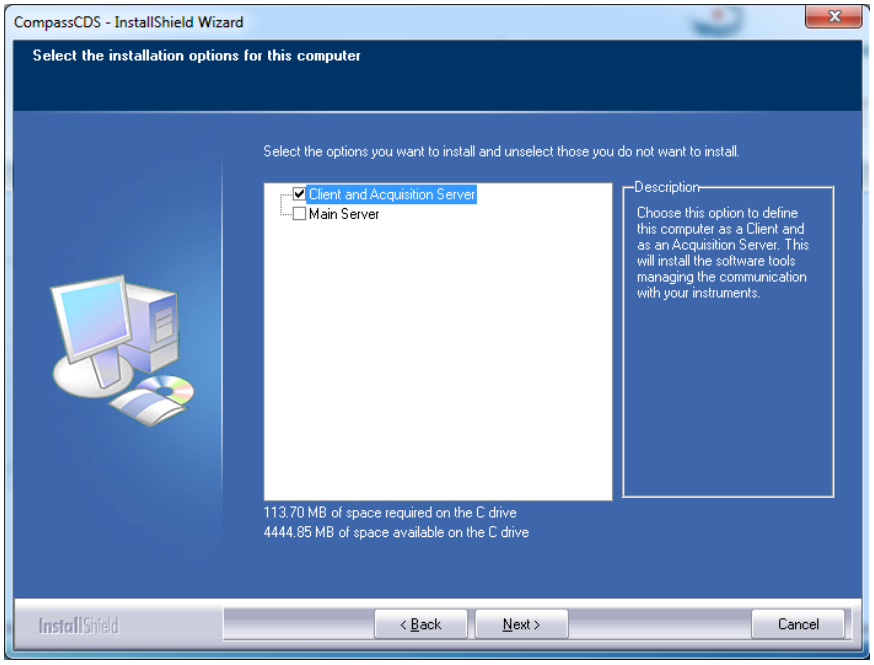
If the client is intended for IPC-MS regulatory support, only a 32-bit Operating system can be used.

Installing CompassCDS client Software on a suitably prepared Windows computer

1. Ensure that the CompassCDS server (already installed) has sufficient Station (computer) and System (instrument) licenses installed to allow for one or more CompassCDS client computer installations.
2. Insert the CompassCDS software media into the client computer, and select the *Install CompassCDS* menu option (shown below). If the installation menu does not load, navigate to the CD drive (usually D:) and select the autorun option.



3. Click Next, Next, Yes to accept the software license terms and then select the Client/Server option and click Next. The Standalone option is only ever used for non-client server CompassCDS installations.
4. Check the Client and Acquisition Server checkbox only and NOT the Main Server option checkbox (as shown below) and click Next.


CompassCDS - InstallShield Wizard
Select the installation options for this computer
Select the options you want to install and unselect those you do not want to install.
Client and Acquisition Server
Main Server
Description
Choose this option to define this computer as a Client and as an Acquisition Server. This will install the software tools managing the communication with your instruments.
113.70 MB of space required on the C drive
4444.85 MB of space available on the C drive
InstallShield
< Back
Next >
Cancel

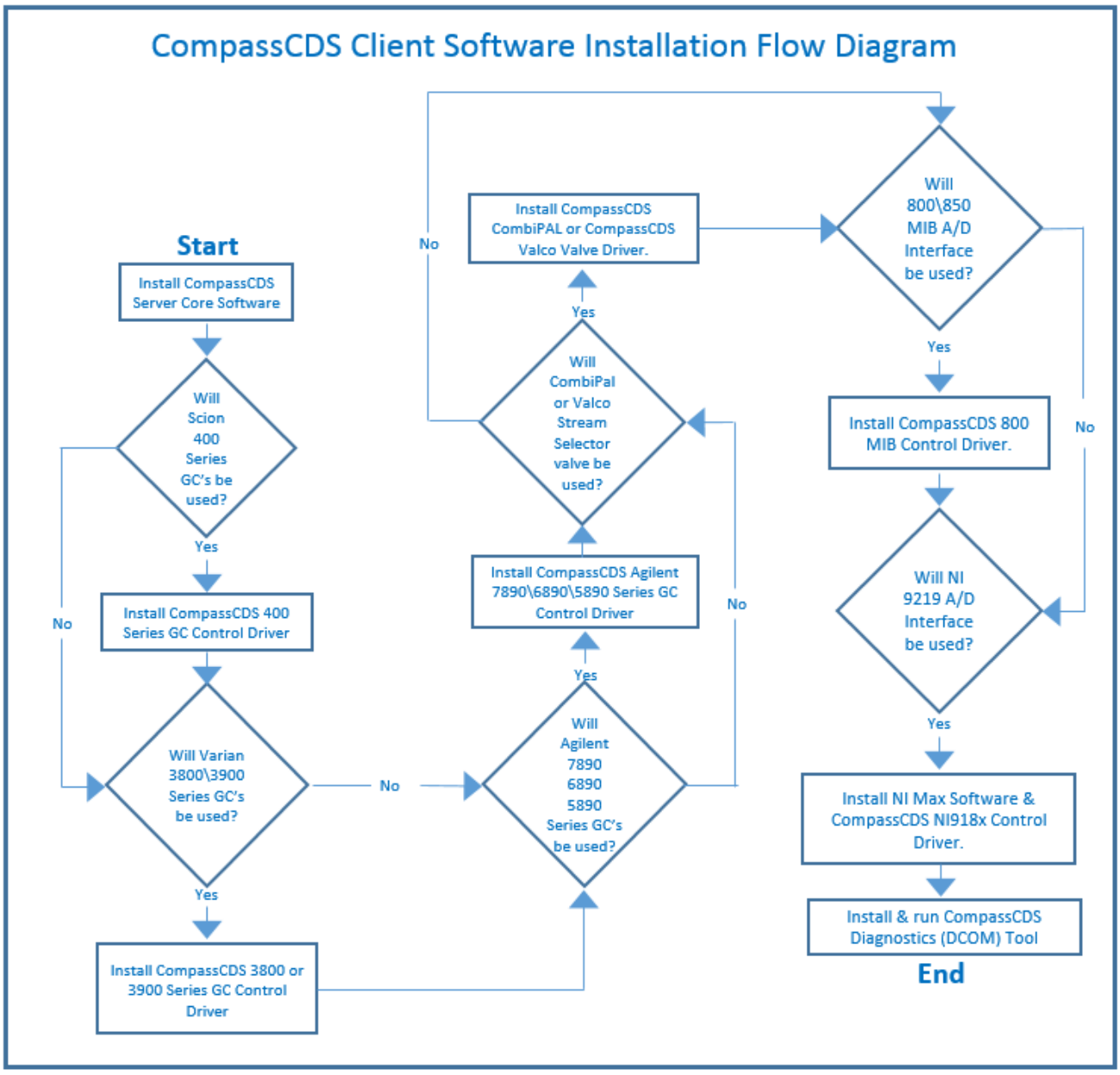
5. Click Next, Next, Next and the CompassCDS software installation will proceed. When prompted, select the restart computer now option and the server will initiate a re-boot sequence.
6. After the computer has completed re-booting, press Control + Alt + Delete keys and log on to the Domain using the administrator login.
7. The CompassCDS client software installation will continue and complete with the following message “Congratulations, you have successfully installed CompassCDS. Click Finish.

8. Log into Compass Configuration Manager from the client computer using:

   User: admin

   Password: compass

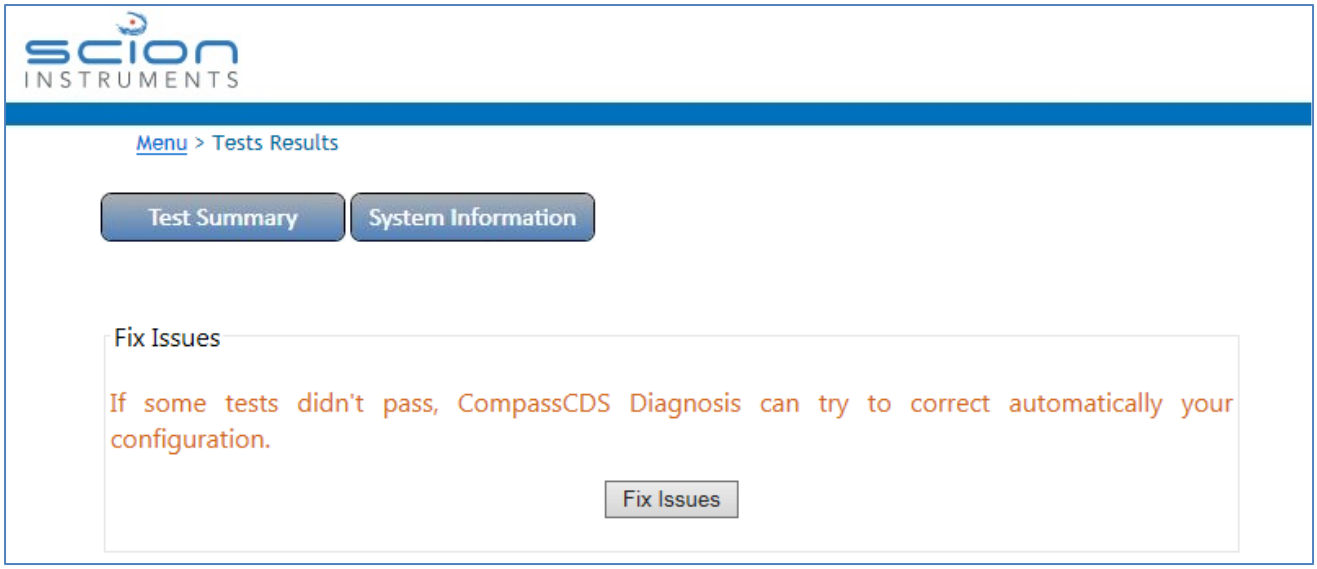
9. Confirm from the top menu in Configuration Manager >Options> Licenses that the serial number entered during the initial part of the install process is listed.
10. Enter any additional Station (computer) and System (instrument) license serial numbers by selecting the Add option.
11. CompassCDS instrument control drivers should now be installed on the CompassCDS client computer even if this this computer has not been designated as an acquisition & control server (which means that it can “own” and control GC and LC instruments) as these drivers are still required to view active acquisitions from CompassCDS client computers. A CompassCDS client software installation flow diagram (see below) indicates the way the instrument control drivers should be installed. To install the CompassCDS instrument control drivers, select the Drivers and Manuals menu option from the CompassCDS install CD and then select the appropriate driver set to install. Enter the appropriate serial number when prompted and let the installation complete.
12. Check that Internet Explorer Active Scripting is enabled (Go to Internet Explorer, Tools, Internet Options, Security, Internet, Custom Level, Active Scripting – Enable).
13. Once the driver software installation has completed, select the Tools and Documentation option from the CompassCDS CD and run the CompassCDS Diagnostics Tool. This tool will install an UltiPro web server as part of the CompassCDS Diagnostics Tool setup.
14. Run the CompassCDS DCOM Tool from the desktop icon and click on the CompassCDS Installation Analysis option. Click on Go and Fix Issues. Close this window.
15. The CompassCDS client software is now installed and this procedure should be repeated for all additional CompassCDS client computers.


CompassCDS Client Software Installation Flow Diagram
Start
Install CompassCDS Server Core Software
Will Scion 400 Series GC's be used?
Yes
No
Install CompassCDS 400 Series GC Control Driver
Will Varian 3800\3900 Series GC's be used?
Yes
No
Install CompassCDS 3800 or 3900 Series GC Control Driver
Will Agilent 7890 6890 5890 Series GC's be used?
Yes
No
Install CompassCDS Agilent 7890\6890\5890 Series GC Control Driver
Will CombiPal or Valco Stream Selector valve be used?
Yes
No
Install CompassCDS CombiPAL or CompassCDS Valco Valve Driver.
Will 800\850 MIB A/D Interface be used?
Yes
No
Install CompassCDS 800 MIB Control Driver.
Will NI 9219 A/D Interface be used?
Yes
Install NI Max Software & CompassCDS NI918x Control Driver.
Install & run CompassCDS Diagnostics (DCOM) Tool
End

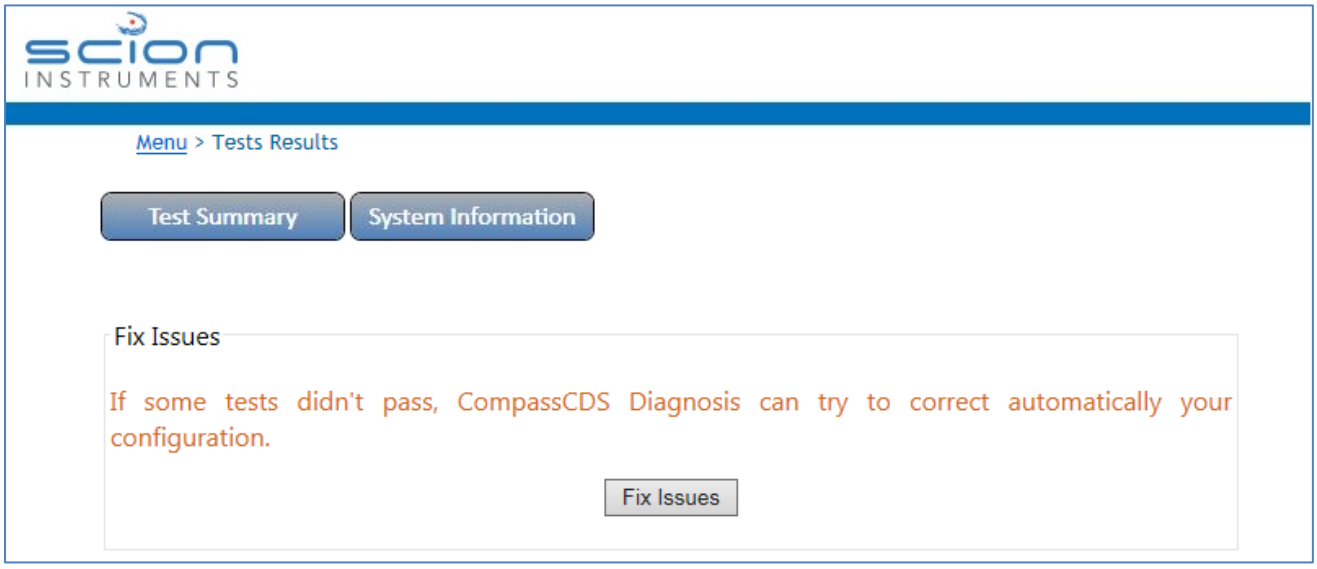
CompassCDS DCOM and Folder Permission Setting Tool

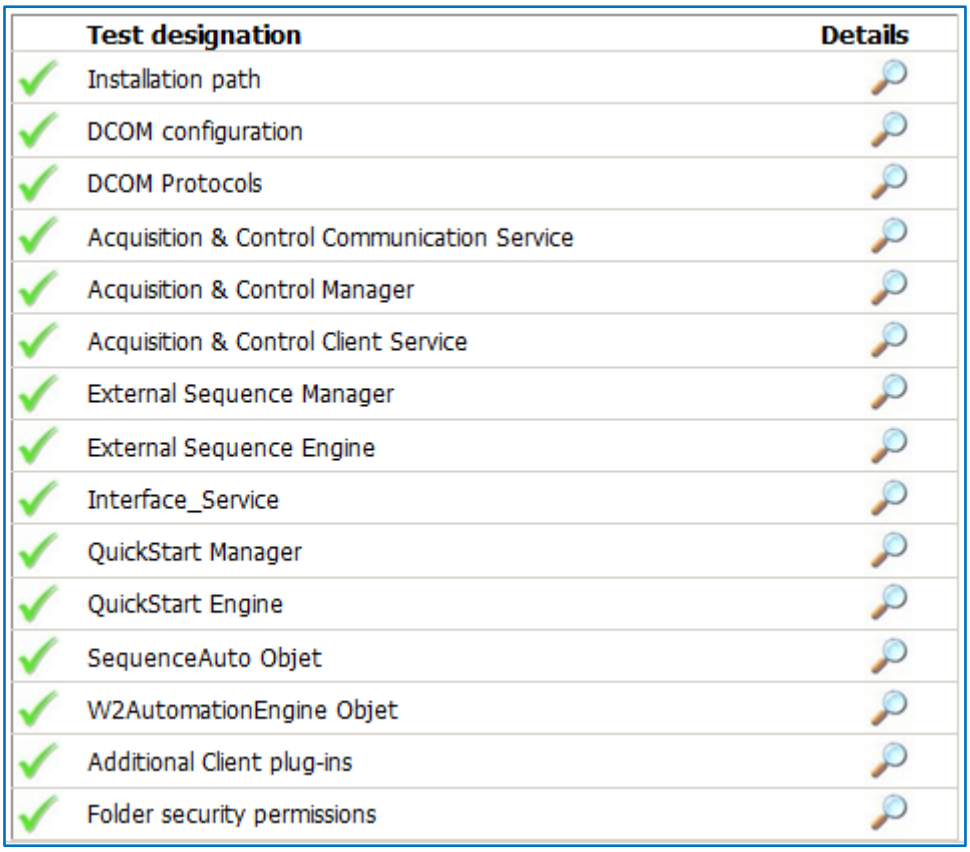
After installing CompassCDS as a networked client server system, it is necessary to set several DCOM and folder permissions on the CompassCDS main server and all the CompassCDS client computers for CompassCDS to be able to control instruments and functional properly. If CompassCDS has been installed as a standalone workstation, it is not necessary to set any DCOM permissions.

An automated software tool has been developed for this purpose. The CompassCDS Diagnostics Tool should be installed and run on the CompassCDS main server and all CompassCDS client computers. This tool is available on the CompassCDS CD in the Tools and Utilities section. This application requires that Windows .Net 3.5 which can also be accessed from the Tools and Utilities section. Once the Diagnostics Tool has been installed, it can be accessed from a desktop icon.



	Test designation	Details
✓	Installation path	
✓	DCOM configuration	
✓	DCOM Protocols	
✗	Acquisition & Control Communication Service	
✓	Acquisition & Control Manager	
✗	Acquisition & Control Client Service	
✗	External Sequence Manager	
✓	External Sequence Engine	
✗	Interface_Service	
✓	QuickStart Manager	
✓	QuickStart Engine	
✗	SequenceAuto Objet	
✗	W2AutomationEngine Objet	
✗	Additional Client plug-ins	
✓	Folder security permissions	





NOTE: It is also possible to set all the DCOM and folder permissions manually if required. The manual DCOM permission setting procedures for Windows XP, Windows 7 and Windows 2003/2008 Server are described in Appendix 1.

CompassCDS Folder Access Permission Configuration

This section provides details about the permission settings associated with the following CompassCDS applications and folders:

NOTE: All of these permissions can be automatically set by installing and running the CompassCDS Diagnostics Tool described in the preceding section of this user guide.

To manually set these permissions, select the appropriate directory in the Windows Explorer, in the popup menu select ‘Properties’, then in the security tab, select the ‘Permissions’ option.

On CompassCDS Workstation and Main Server computers:

All the permissions can be RX except for the system TEMP directory (i.e., <CompassCDS>\Server\TEMP) that should have the RWXD permissions for the users/groups INTERACTIVE, SYSTEM, NETWORK, ANONYMOUS LOGON, DOMAIN USERS.

More precisely for the '****CompassCDS\SERVER' folder, the permissions settings are:

Directories or files	INTERACTIVE, SYSTEM, NETWORK, ANONYMOUS LOGON, DOMAIN USERS
*.EXE; *.DLL; *.CHM	RX
All other files	RWX
\TEMP; \DEVICES; \LOGS; \DATA_SHARED	Modify
\CFG	RW

For users who access this folder over network, permissions must be set in the folder share. Select the '****CompassCDS\SERVER' folder, in context menu select PROPERTIES, then the 'Sharing' tab. Click on the 'Permissions' button and add 'Everyone' in 'Full control' in the list.

On the Data Directory:

The data directories can have the following permission settings if you don't need to overwrite DATA files:

- Administrators Full control
- DOMAIN USERS RWL
- NETWORK RWL
- SYSTEM RWL
- INTERACTIVE RWL
- ANONYMOUS LOGON RWL

The data directories can have the following permission settings if you need to overwrite DATA files:

- Administrators Full control
- DOMAIN USERS RWLD
- NETWORK RWLD
- SYSTEM RWLD
- INTERACTIVE RWLD
- ANONYMOUS LOGON RWLD

With R=Read, W=Write, L=List Folder Contents, D=Delete, X=Execute

For users who access the 'DATA' folder over a network, permissions must be set in the folder share. Select the 'DATA' folder, in context menu select 'PROPERTIES', then the 'Sharing' tab. Click on the 'Permissions' button and add 'Everyone' with 'Full control' in the list.

On Printer:

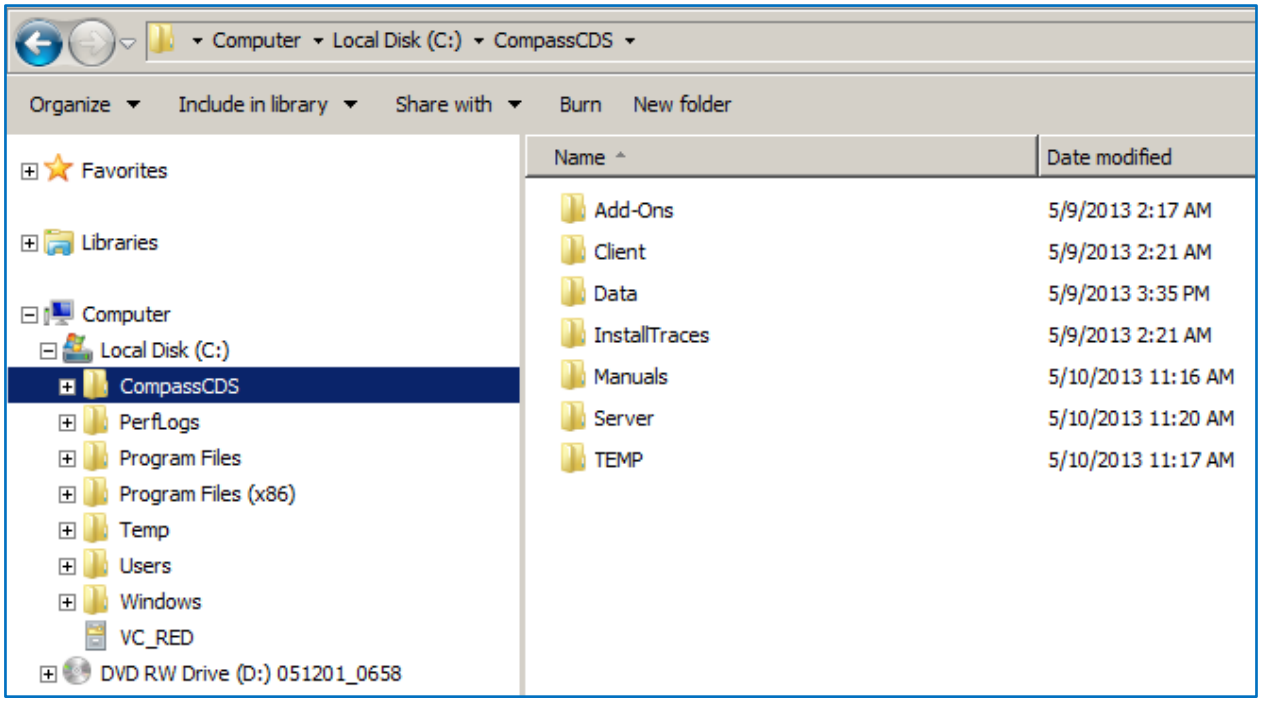
If report printing is done while running remote sequences, check that the following security permissions are present in the default printer properties.

- DOMAIN USERS: Print + Manage Printers + Manage Documents
- SYSTEM: Print + Manage Printers + Manage Documents
- INTERACTIVE: Print + Manage Printers + Manage Documents

CompassCDS File Type Descriptions

This section describes the content of the **CompassCDS** folder and subfolders created during the software installation and provides information on the main files.

The C:**CompassCDS** directory content is accessible from Windows Explorer:



The C:\CompassCDS**Add-Ons** folder contains the CompassCDS Plug-in option installations.

The C:\CompassCDS**InstallTraces** folder contains the complete log generated during a CompassCDS installation. However, if the install ends abruptly due to a problem on the computer, the logs will be located in the following directory:

“C:\DocumentsandSettings\Admin\LocalSettings\Temp\<sessionGUID>\<applicationGUID>” where:

<sessionGUID> differs every time an InstallShield session is launched, even if it is dealing with the same setup: for example, {7A9045C0-59AE-4B1D-AE8D-B4887E3AAA9B}

<applicationGUID> is constant for a product to install:

For CompassCDS: {490A76B0-59E3-11D7-9152-0050042084E2}

The C:\CompassCDS**Client** folder contains:

- CompassCDS.exe, the CompassCDS executable file.
- CompassCDS report editor.exe, the CompassCDS report manager executive file.
- W2AutoEngine.exe program used to print the reports of the sequences launched by the Remote Sequence Manager.
- The Remote sequence exe files: SeqClient.exe (the client), SequenceManager_Service.exe and SequenceEngine_Service.exe (the services exe files).
- All the DLLs related to the above programs.

The C:\CompassCDS**Data** folder contains chromatogram examples and some predefined report styles:

- *.METH: the method files.
- *.DATA: the chromatogram files.
- *.SEQU: the sequence files.
- *.REPL: the reprocessing list files.
- *.SUMR: the summary report files.
- *.STYL: the report style files.
- Other type of files:
    - ~$"Name of the file".*: lock files used to prevent the use of the same file by different users simultaneously.
    - CACHE_*.TXT: Caches used to speed up the display of the file lists in the open dialog of CompassCDS.
    - *.tmw: temporary files used when an acquisition is started.

The C:\CompassCDS**Manuals** folder contains all the user guides for CompassCDS.

The C:\CompassCDS**Server** folde**r** contains the following files and subfolders:

- configurationmanager.exe, the CompassCDS configuration and maintenance manager executable file.
- AcqClientSvr.exe, AcqManSvr.exe, AcqSystSvr.exe
- BOOTPSVR.exe

The **CFG** folder contains the configuration files for all systems configured on that computer (Only for the acquisitions servers).

The **CMDATA** folder contains all the Nexus database tables and parameters contained in the CompassCDS Configuration Manager application.

The **CSDATA** folder contains columns and solvent preferences.

The **Data shared** folder file contains:

- The FormatLib.dat: which is the file containing all the peak, group and chromatogram formats defined in CompassCDS.
- The .REPO files represent the repositories created in CompassCDS (variables creation).
- All the .REGC files which stores the users preferences
- Some .INI files which store the last Suffix ID used for each Group/Project/System set.

The **Devices** folder, contains the driver .dll files of all the configured systems.

The **IQOQ** folder contains all the documents and data files required to qualify CompassCDS installation and operation in regulated environments.

The **LOGS** folder contains .txt information, warning, error and other diagnostic log files that are produced when CompassCDS is operating, controlling instruments and acquiring data. These log files are automatically archived in the C:\CompassCDS\Server\Logs\LogArchives folder once these reach 2 GB in size and new logs are immediately generated.

The **TEMP** folder, contain a sub-directory for each acquisition system, and each directory stores some temporary files used for the acquisition (*.HTML files: store a HTML representation of the control method, this HTML file will be part of the DATA file at the end of the run (on CompassCDS server) and *.tmp: temporary files used when an acquisition is started (on acquisition server).

Windows Services

This section describes the different Windows services that are installed and used by CompassCDS: Acquisition & Control Manager.

(Exe path is \CompassCDS\Server\AcqManSvr.exe):

- This service is the “control tower” of the CompassCDS system.
- Stopping this service also stops all the running systems of the computer.

Acquisition & Control System – “Name of the system”

(Exe path is \CompassCDS\Server\ AcqSystSvr.exe):

- One service is declared for each CompassCDS systems.
- Stopping one of these services stops all activity on the system.

BOOTP Service

(Exe path is \CompassCDS\Server\bootpsvr.exe):

> This service is the main service which handles the BOOTP devices that require an IP address to be dynamically assigned from a BootP server. As most modern instruments have statically assignable IP addresses and very few devices still require this service, it is installed but is turned off (disabled) by default in the Windows Services and needs to be enabled when it is required for use on a particular acquisition and control server.

NexusDB_Server

(Exe path is \CompassCDS\Server\CM DATA\nxserver.exe):

- It is MANDATORY to leave this service running all the time.
- This is the main service which manages access rights for the users, the status of the CompassCDS systems.

External Sequence Manager

(Exe path is \CompassCDS\Client\ SequenceManager_Service.exe):

- This service is the control tower of all sequence engine services running on the computer.

External Sequence Engine – “Name of the system”

(Exe path is \CompassCDS\Client\ SequenceEngine_Service.exe):

- One of these services is declared for each CompassCDS systems.
- It handles the remote sequence launched from the remote sequence client.

Routine CompassCDS System Maintenance

The recommended maintenance: As the files generated are quite small and numerous, use a disk defragmentation tool.

Once a month, delete all (except the one of the current day):

- *.tmw in the data directories.
- Delete all files in the \CompassCDS\SERVER\TEMP directory of the acquisition server.
- Delete all files in the \TEMP directories.

Recommended backup and recovery procedure for CompassCDS Workstation and Main Server Installations

CompassCDS Backup Procedure

Folders and files that need to be backed up for later use, should a re-installation of the CompassCDS software be required, include the following:

C:\CompassCDS\Server\CFG

The CFG folder contains the configuration information of all the chromatographic systems listed in Configuration Manager. This folder only needs to be backed up if the CompassCDS computer has been designated an acquisition server and this folder contains one or more .CFG files.

C:\CompassCDS\Server\CMData
The CMData folder contains all the parameters contained in the CompassCDS configuration Manager. Before backing up the CMData folder, it is necessary to stop the NexusDB Server service which is located in Windows Services. Once the backup has been completed, this service should be restarted. All the .NX1 filed contained in this folder should be backed up.

C:\CompassCDS\Server\CSData
The CSData folder contains all the column and solvent database information and only needs to be backed up if either of these applications is being used.

C:\CompassCDS\Server\Data_Shared
The Data_Shared folder contains the following file types that require backup:

- The .REPO files that represent the custom variable repositories created in CompassCDS
- All the .REGC files that store user preferences
- Certain .INI files that store the last Suffix ID used for each Group/Project/System set.

C:\CompassCDS\Data (or any other folder\mapped drive in\on which CompassCDS .DATA, .METH, .SEQU, .REPL, .CALB, .SUMR and .STYL files are being stored).

CompassCDS Recovery/Restore Procedure

If re-installation of CompassCDS becomes necessary, the existing CompassCDS software installation should be uninstalled using the Windows Add/Remove or Uninstal. Once the uninstall has completed the computer should be rebooted and then the existing C:\CompassCDS folder (or equivalent path) should be deleted.

A new CompassCDS installation should then be initiated either as a standalone workstation or CompassCDS main server and it is essential that the installation folder path be exactly the same as the path from the previous install. At least one reboot of the computer will be required during this installation. Once the install has completed, stop the NexusDB Server service in the as described previously and replace the following files with those from the backup:

1. Replace all .CFG files in the newly created C:\CompassCDS\Server\CFG folder with those from the backed up C:\CompassCDS\Server\CFG folder.
2. Replace all .NX1 files in the newly created C:\CompassCDS\Server\CMData folder with those from the backed up C:\CompassCDS\Server\CMData folder
3. Replace all .NX1 and other files in the newly created C:\CompassCDS\Server\CSData folder with those from the backed up C:\CompassCDS\Server\CSData folder.

4. Replace all .REPO, .REGC and .INI files in the newly created C:\CompassCDS\Server\Data_Shared folder with those from the backed up C:\CompassCDS\Server\Data_Shared folder.
5. Copy all the .DATA, .METH, .SEQU, .REPL, .CALB, .SUMR, and .STYL files from the backed up **C:\CompassCDS\Data** (or any other folder\mapped drive) into the newly created C:\CompassCDS\Data (or equivalent) folder.

The NexusDB Server service can now be restarted and it should be possible to log into CompassCDS and Configuration Manager using any of the usernames and passwords from the previous instance of CompassCDS.

CompassCDS Troubleshooting Tips

This section describes several known errors observed after installing CompassCDS and ways to avoid them.

Networking

Network spanning trees can, on rare occasions, affect CompassCDS operation (causing Remote Sequence hangs). If this occurs, simply disabling this network feature should resolve the issue.

CompassCDS installation fails if more than one network card is activated (error “Lhotse failed to initialize, code -13” during the installation). Only one NIC card must be enabled to install CompassCDS correctly.

101 Station Systems Error Caused by corruption of Compass licensing during the installation.

Folder permissions error after installing a C/S Permissions for folder directories not set correctly.

Frequent disconnects of instruments – Anti Virus applications or Firewalls.

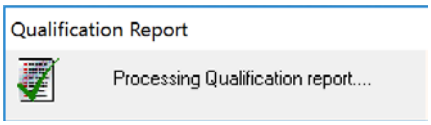
CompassCDS Software Installation Qualification

It is possible to validate the installation of the CompassCDS Workstation, Server, Client or any Instrument Control driver software. The validation program is installed automatically during a CompassCDS installation.

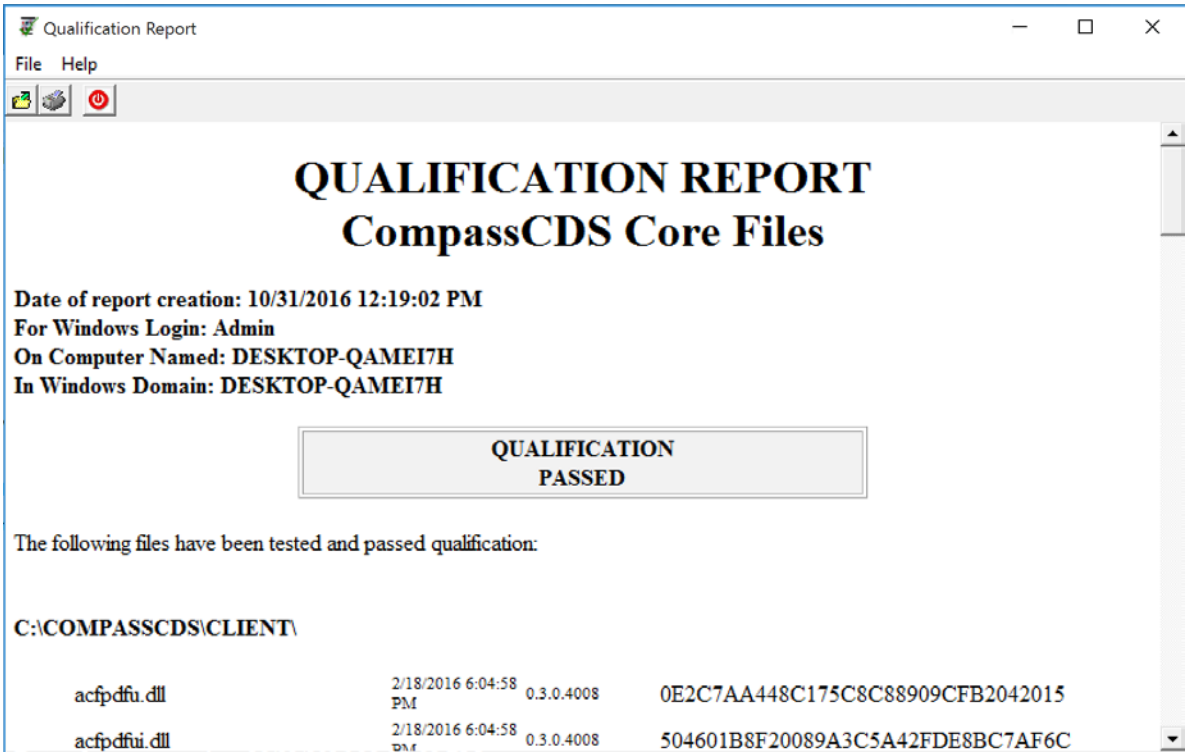
After CompassCDS installation, Validation Reports for the core and all instrument control drivers can be found either in a specific subfolder belonging to the CompassCDS menu (Windows 7) or as part of the CompassCDS folder (Windows 10) in the Windows Start Menu:

Select the software installation you want to validate (CompassCDS Core or Driver).

The validation program will launch. Wait until the following screen disappears.



The read-only validation report is then displayed on the screen.

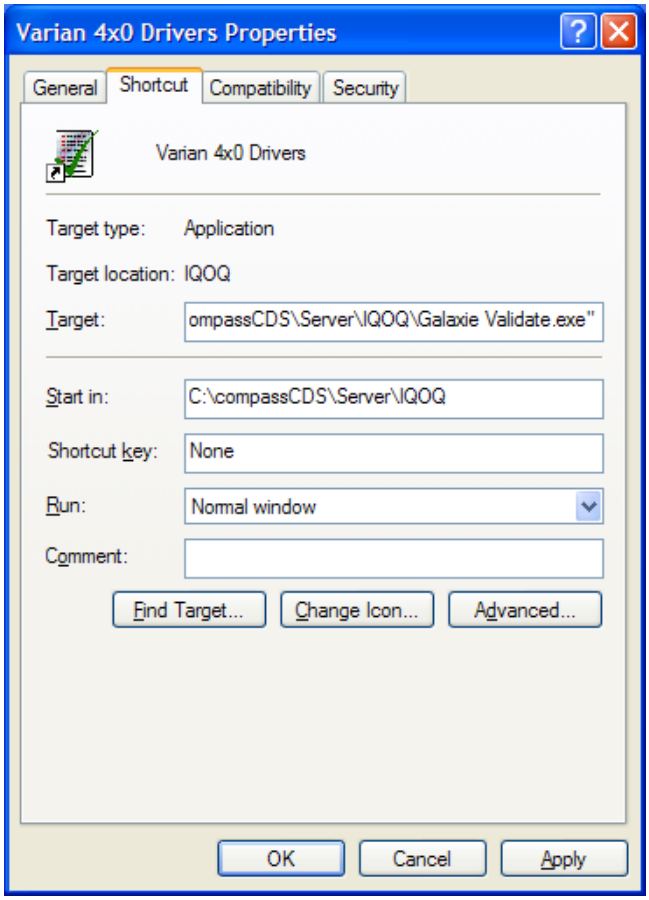


These reports can be printed and are automatically saved in <CompassCDS>\Server\IQOQ\.

After installing non-Scion Instruments drivers on CompassCDS (drivers from Agilent, Thermo, etc.) the installation validation of these drivers cannot be executed. This is caused by an invalid shortcut in the start menu. Execute the following steps in order to fix this problem:

1. Locate the shortcut to the validation report of the driver in the Windows start menu. It is possible that it is located under “GALAXIE (Chromatography)”.

2. Right-click on the shortcut and select Properties:



3. In the target edit field locate “Galaxie Validate.exe” and change it to “CompassCDS Validate.exe”.
4. Click OK.

CompassCDS Instrument Control Drivers

This section describes the principles and operation of the CompassCDS instrument control drivers.

Principles

Each CompassCDS controlled chromatographic system can comprise one or several modules.

For instance, a system controlling a Scion 456 GC with an 8400 autosampler will be composed of:

- Scion 456 GC only as the 8400 control is an integral part of the 456 GC control driver.

Whereas, if a Scion 456 GC was being configured for manual injection only, the system would be composed of:

Scion 456 GC control driver

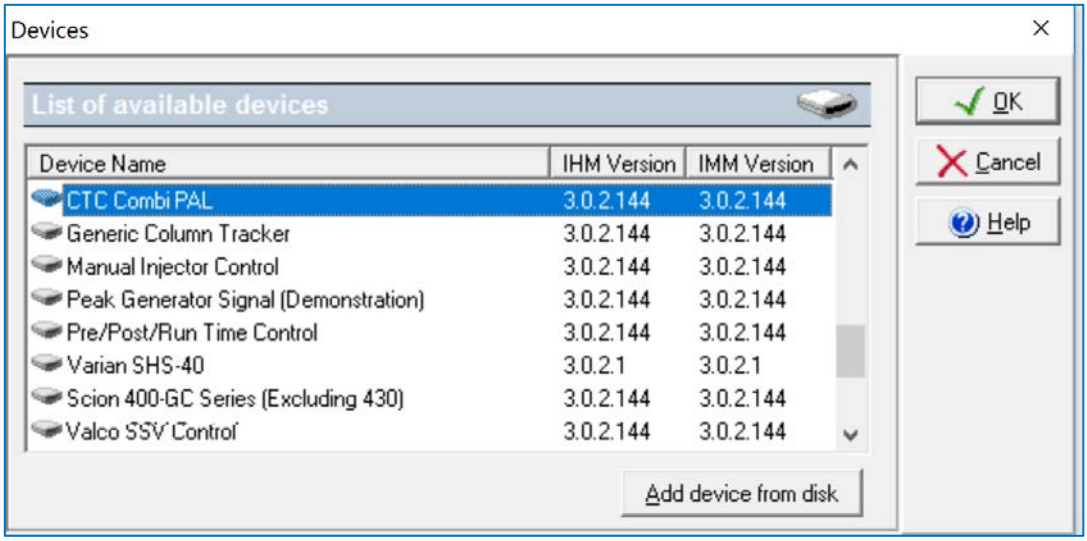
Manual Injector control driver

Each CompassCDS control driver comprises two elements:

- The *_IMM.dll file which contains all the code required to control the device.
- The *_IHM.dll file which contains all the screens necessary to configure, build methods, and display the status of the device.

File Locations

In CompassCDS Configuration Manager (menu “Option | Devices…”), the screen displays all the available modules for the system:



The control driver DLLs for all CompassCDS controlled are stored in the \CompassCDS\Server\Devices folder (both the *_IMM.dll and *_IHM.dll files

Instruments Control Driver Installation

Control drivers for the following CompassCDS controlled devices can be installed from the CompassCDS media:

- Scion 400 Series GC – Control of 456, 436, 450 and 430 with integrated 8400 & 8410 autosampler control
- Varian 3800 & 3900 GC – Control of legacy Varian 3800 and 3900 with integrated 8400 & 8410 autosampler control
- CTC Combi PAL
- Scion SHS-40 Headspace
- Valco SSV
- National Instruments 9219 Analog to Digital, 9481 Relay & 9401 TTL I/O
- Varian STAR 800/850 MIB
- Agilent 5890 GC – Control of HP 5890 including 7673 headspace Autosampler
- Agilent 6890 GC – Control of HP 6890 & 6850 GC including 7683 and 7693 autosampler and 7694 headspace autosampler
- Agilent 7890 GC – Control of Agilent 7890 A/B GC including 7693 autosampler and 7694 headspace Autosampler
- Agilent 1260 LC – Control of HP 1100, Agilent 1200, and Agilent 1260 LC including Infinity I, II series LC modules

In addition to this list, several control drivers are automatically installed during an initial CompassCDS installation. These include:

- Manual Injector
- Pre-Post-Run Control
- Column tracker

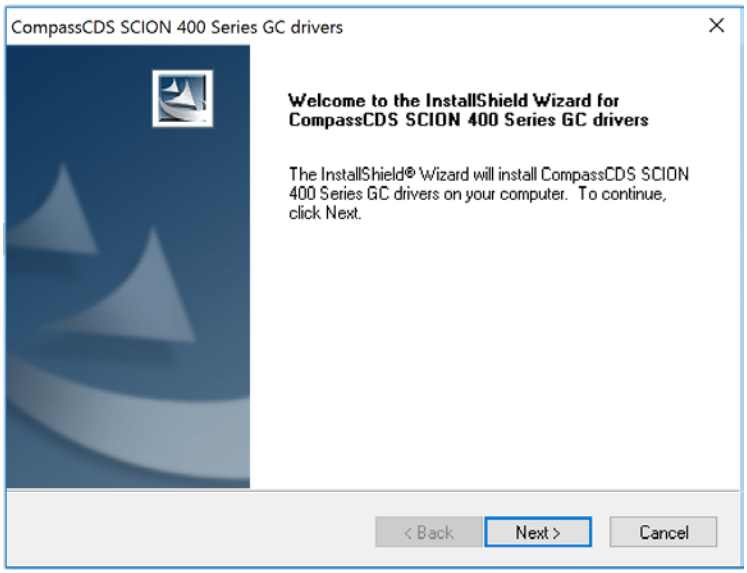
Scion Instruments 400 Series GC

Installing the Driver Software

The CompassCDS core software must already be installed before installing the control driver software.

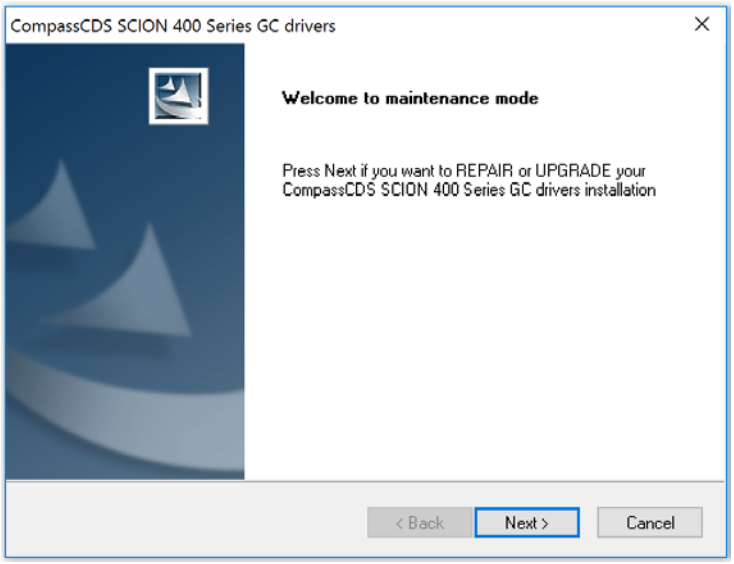
Users must have local administrator rights to install this driver, or domain administrator rights if the computer is part of a Windows domain.

Insert the CompassCDS DVD into the CD/DVD drive, and the DVD browser will start automatically. If it does not, launch the browser by running ‘autorun.exe’ from the root directory of the DVD, or execute control driver installation directly from the Driver subdirectory by running the ‘setup.exe’ file located the instrument subfolder.


CompassCDS SCION 400 Series GC drivers
Welcome to the InstallShield Wizard for CompassCDS SCION 400 Series GC drivers
The InstallShield® Wizard will install CompassCDS SCION 400 Series GC drivers on your computer. To continue, click Next.
< Back
Next >
Cancel

Click on the ‘Next’ button, read and accept the ‘License Agreement’ and enter the control driver ‘Serial Number’ in the corresponding field. The serial number is provided on the control driver serial number card and is different from the CompassCDS core software serial number. Note that all serial numbers are case sensitive.

Press the ‘Next’ button and click on ‘Finish’ at the end of the installation. If you want to reinstall or upgrade control drivers, it is necessary to run the setup once again.


CompassCDS SCION 400 Series GC drivers
Welcome to maintenance mode
Press Next if you want to REPAIR or UPGRADE your CompassCDS SCION 400 Series GC drivers installation
< Back
Next >
Cancel

Press ‘Next’ and the control drivers will be automatically reinstalled or upgraded. Click on ‘Finish’ at the end of the installation to exit the maintenance mode.

To see which drivers are installed select ‘Options’ from the CompassCDS Configuration Manager main menu and select ‘Devices’. The button

can be used for manually installing beta or pre-release drivers. Use this button only when directed by a technical support representative.

BOOTP Server Configuration

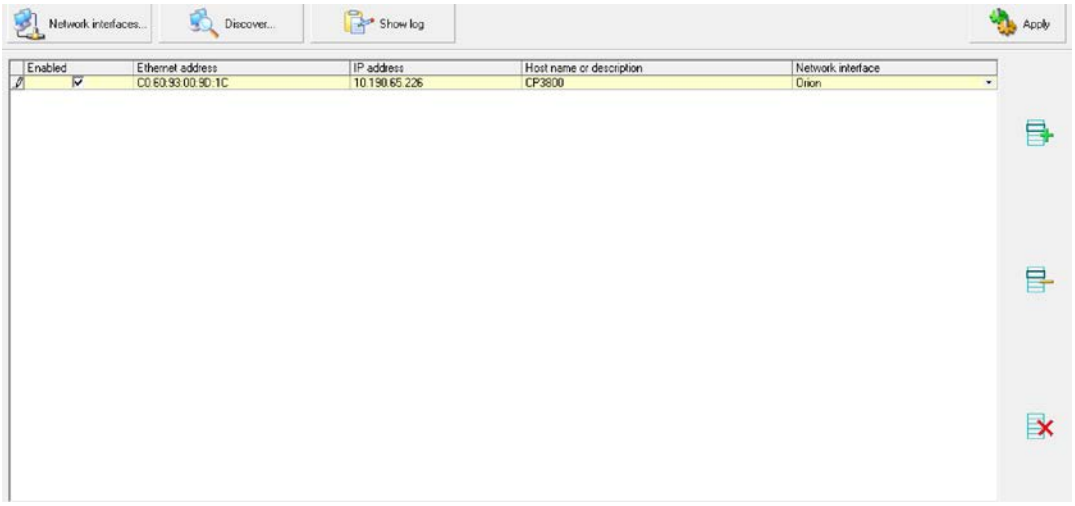
A BOOTP Server is used to send IP addresses to TCP/IP devices.

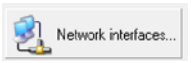
The BOOTP Server lists Ethernet addresses along with the IP addresses that are to be assigned to the corresponding devices.

1. Enable the installed BOOTP Service from Within Windows Services by right clicking on the BOOTPservice and selecting Properties and then Startup Type – Automatic,

Start the BOOTP Server Configuration tool in the CompassCDS Configuration Manager by clicking on the icon

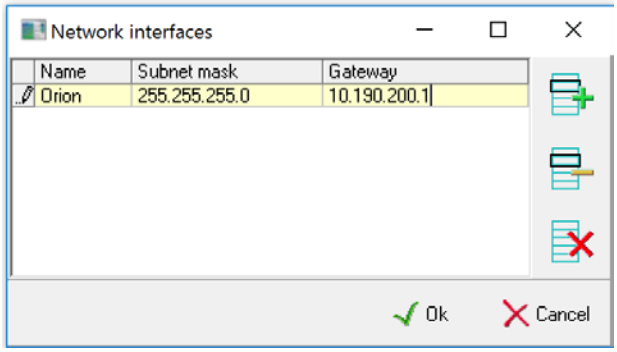
in the Tools section or in the menu Options click on BOOTP configuration. The following screen appears:



Click the 

button to declare the parameters of the network where the instruments and the BOOTP server are located.

The following screen appears:



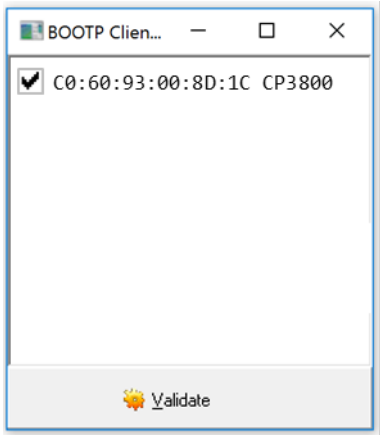
Enter a ‘Name’ for the network card, the ‘Subnet mask’ and ‘IP Gateway’ (optional) addresses.

More than one network card may be declared by clicking on . Selected lines can be deleted by clicking on . All the lines can be deleted by clicking on .

Click on the

button and the BOOTP server will enter discovery mode, during which will automatically find and list the MAC addresses of all the instruments which are broadcasting IP Address requests

The following screen appears:

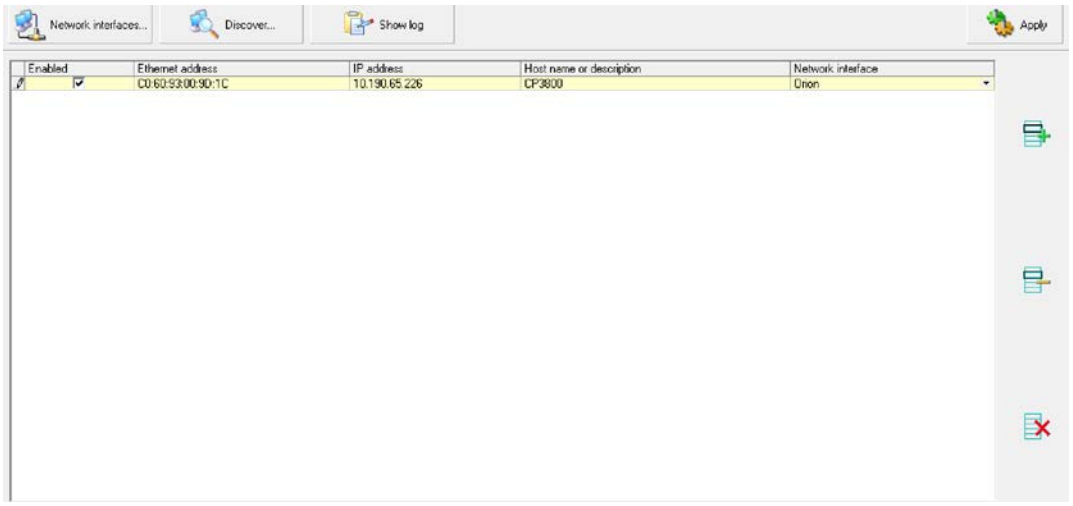


Note: If the required instruments are powered on, and their MAC addresses do not appear after a few minutes, ensure that the Windows Firewall and any anti-virus software installed on the computer is disabled as these will prevent BootP broadcasts from reaching the BootP server. It is also possible that Ethernet switches can sometimes prevent IP broadcasts from reaching the BOOTP Server and these should be reset (when possible).

Once the correct MAC address and been selected, click on the

Button.

The corresponding instruments are then listed in the main screen:



Complete the mandatory fields by entering the IP address assigned to the selected instrument, its Name or Description and the Network interface previously declared and assigned to the instrument.

By clicking on the button, an instrument can be declared manually.

In this case, enter the Ethernet address which allows the computer to locate the instrument and to upgrade the IP address without reloading it every time it changes.

Complete the other fields (IP address, Name, etc.) as described above.

Delete the selected line by clicking on or to clear all lines in the table.

Click on the

button to see details about the requests sent by the instruments, the answers of the BOOTP server, or the errors.

When all the instruments have been correctly declared, click on ‘OK’, or ‘Apply’ to validate.

NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software but is turned off by default and must be enabled for use in Windows Services.

System Configuration

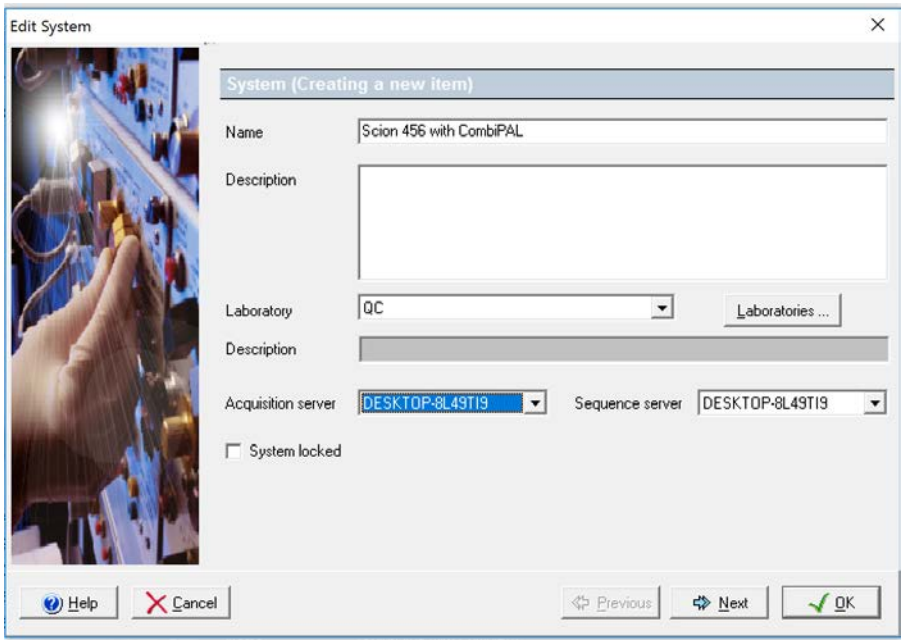
Scion Instruments GC Systems

Example: Combi PAL Autosampler, 456 GC connected via an Ethernet switch

To configure the system shown above, complete the following steps:

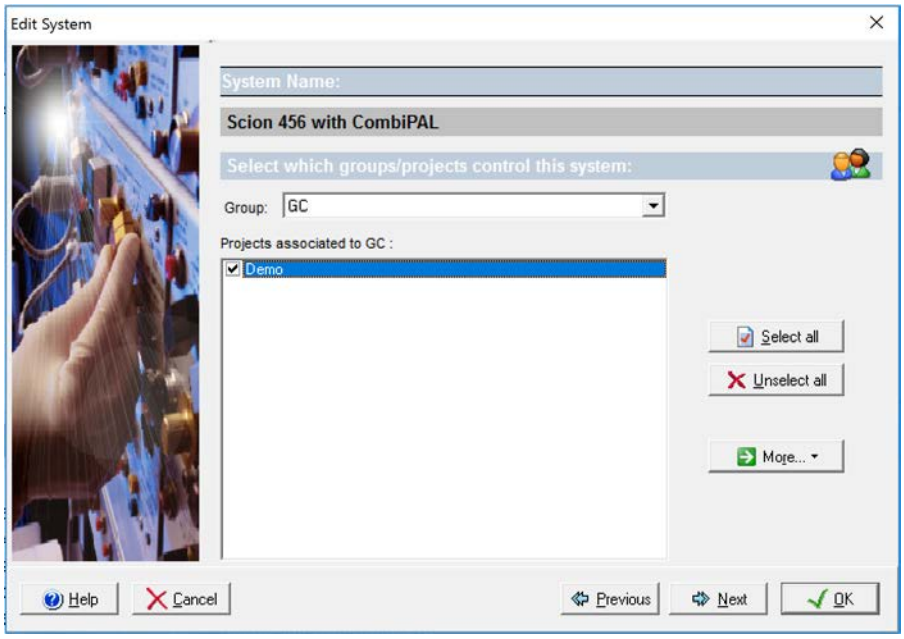
Setup the BOOTP or DHCP server if the 456 GC does not have a fixed IP address (recommended), or set it directly on the GC.

In the CompassCDS Configuration Manager, create a new system. The following screen will be displayed.

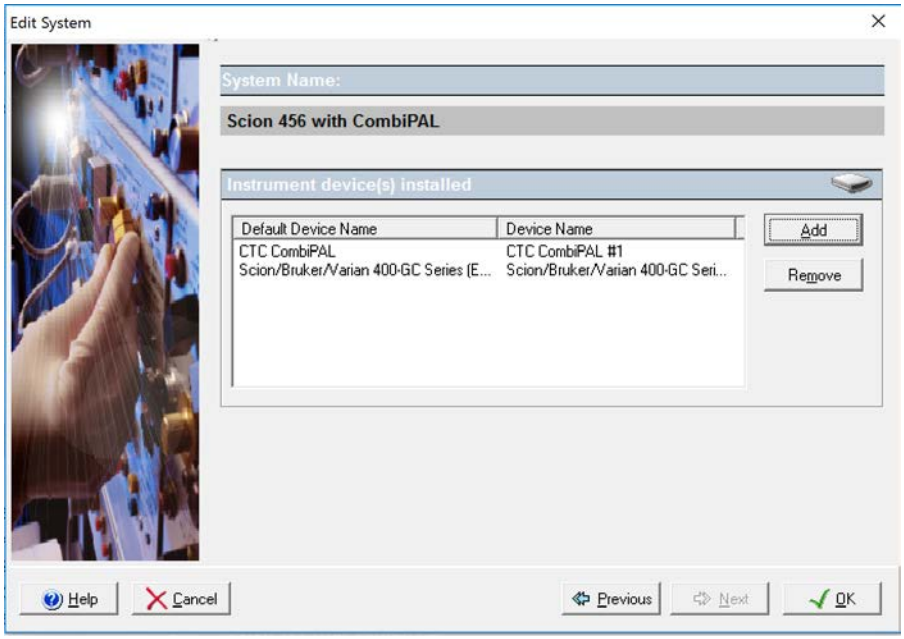


Enter the ‘Name’ of the system, select in the ‘Acquisition server’ and ‘Sequence server’ the name of the acquisition server and the name of the sequence server. Then click on ‘Next’.

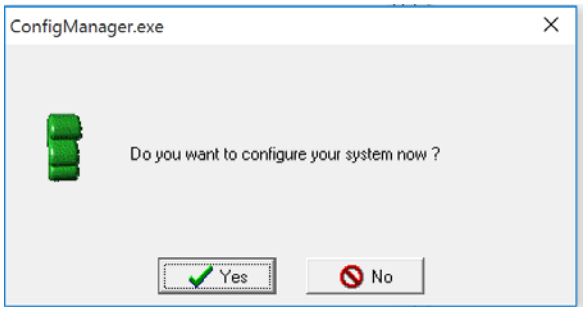
In the following screen, associate one or more project(s) to the system and click on ‘Next’. If no groups/projects are defined, click on ‘Next’.



To configure that system, two device drivers must be installed; the Combi PAL (which represents the injector object) and the 456 GC (which represents the channel object). Click on the ‘Add’ button, select in the ‘Device Type’ list CTC Combi PAL and press ‘OK’. Repeat the same operation but this time select in the ‘Device Type’ list Scion/Bruker/Varian 400 GC-Series Gas Chromatograph. When these two devices have been added, the screen should appear as below.



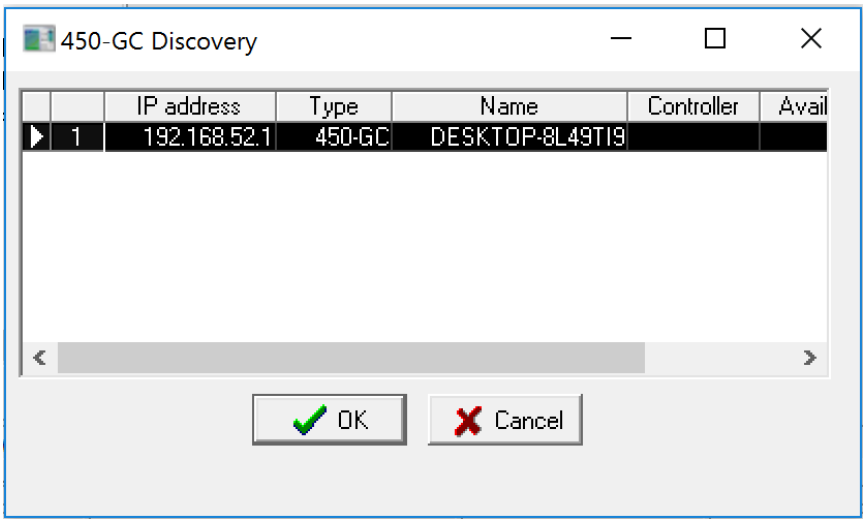
Click on the OK button and answer ‘Yes’ to the question: "Do you want to configure your system now?"



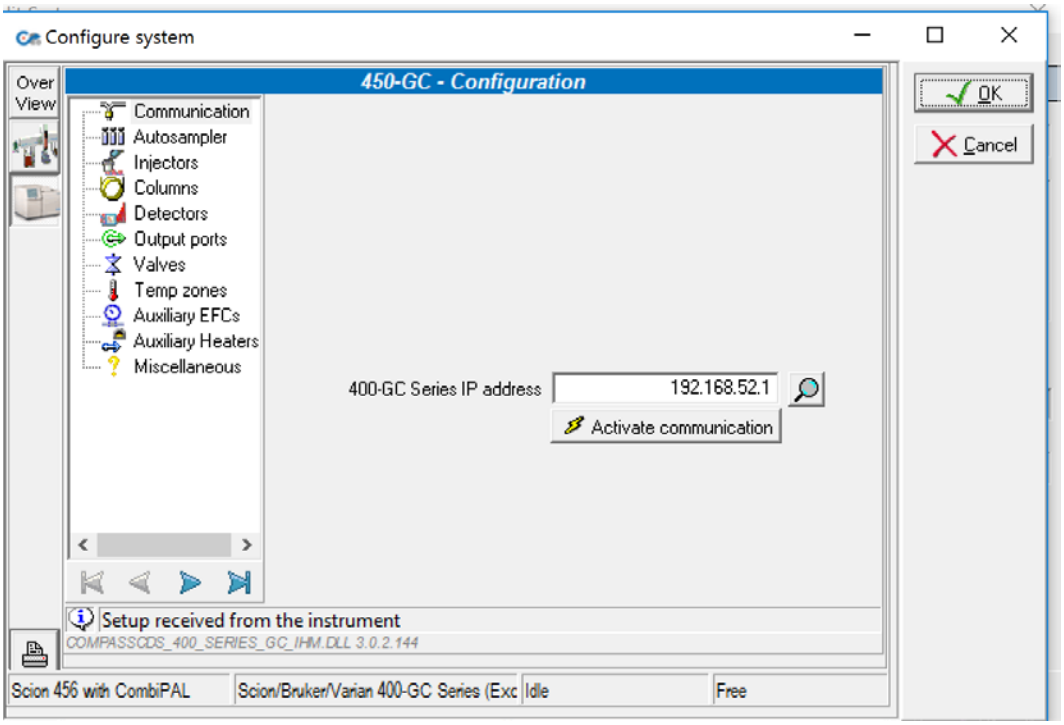
In the next screen, click on the ‘Combi PAL’ icon and click on the ‘Communication’ tab. Select ‘Local serial port’ and the corresponding com port number. Press the ‘Activate Communication’ button.

If the communication is successful, the following progress bar should appear on the screen.

Press the ‘456’ icon and click on the ‘Communication’ tab. Type the GC IP address in the ‘GC name or address’ field or click on the magnifying glass to search all the 456 connected to the network.



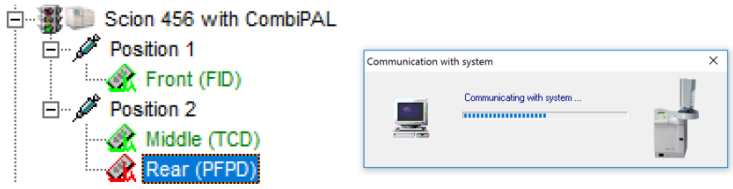
Select the correct GC and click on ‘OK’. Then press the ‘Activate communication’ button. If the communication is successful a message should appear at the bottom of the configuration screen "Setup received from the instrument" (see below).



NOTE: It is advisable to use fixed or static IP addresses to communicate with instrument instead of BOOTP whenever possible.

Click on the ‘OK’ button to finish the configuration of the system.

Finally stop the system by right clicking on its name in the organization view. Then right click again and press start. It is now possible to configure the Overview by going back in the configuration of the system.



For other instrument setup and configuration please refer to the specific instrument control driver user guide.

Checklist for CompassCDS Installation

The following list guides you into CompassCDS installation. It lists the pre-installation requirements (firewall, antivirus, etc.) that are required to successfully install the Scion Instruments CompassCDS Software, as well as the actions to perform after the installation to set correct configuration.

Before launching CompassCDS installation:

- ☐ Ensure the computer/server in part of a Domain and/or the installer has sufficient rights to access all the folder options.
- ☐ Allow only one network card to be enabled during the installation.
- ☐ De-activate all Windows and Third Party Firewalls.
- ☐ De-activate the Automatic Windows updates to avoid the automatic reboots during a sequence, or a single acquisition.
- ☐ Set “Windows only” for the DEP (Data Execution Prevention) for computer/server under Windows 7, 10, and Windows 2008 R2, 2012 R2, and 2016 server
- ☐ De-activate all Power saving options (Hard drive, Wait, Disable Hibernate)
- ☐ De-activate the network card power saving option.
- ☐ De-activate the Anti-Virus software just before the launch of the CompassCDS installation, and during the CompassCDS Installation.
- ☐ Install CompassCDS

After CompassCDS Installation:

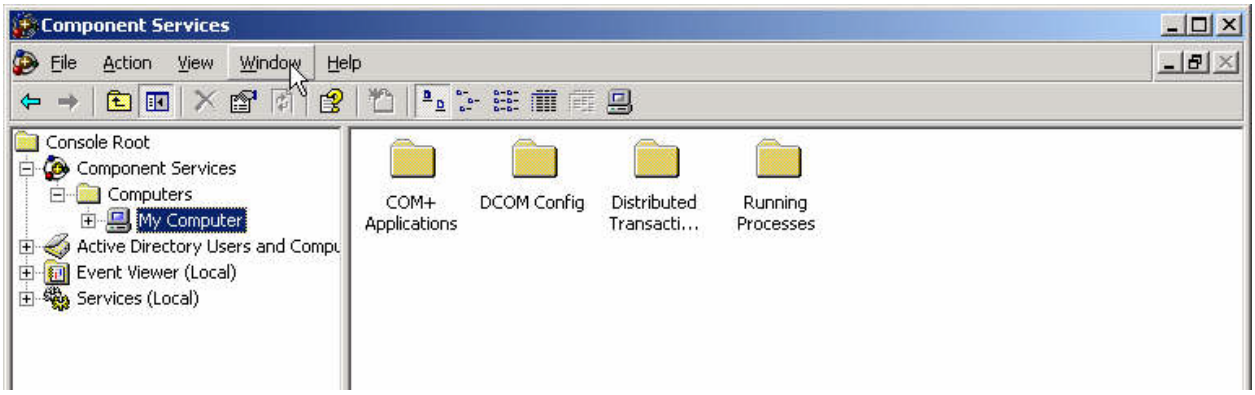
- ☐ Set the Directory rights according to the Installation Guide. Use the CompassCDS Diagnostic Tool.
- ☐ Activate the Anti-virus software, but exclude the CompassCDS folder from being scanned.
- ☐ Complete all the settings that need to be done according to the Installation Guide.
- ☐ Reconnect/Enable the other network cards if present.
- ☐ Reboot the computer.

Appendix 1

DCOM Configuration under Windows 2003 Server

Connect under the Windows session as a local administrator in the ***START*** menu, in the ***RUN*** part enter ***DCOMCNFG***.

The following window is opened:



Right click on *My Computer* and select Properties. A window is opened with six tabs:

General

Options

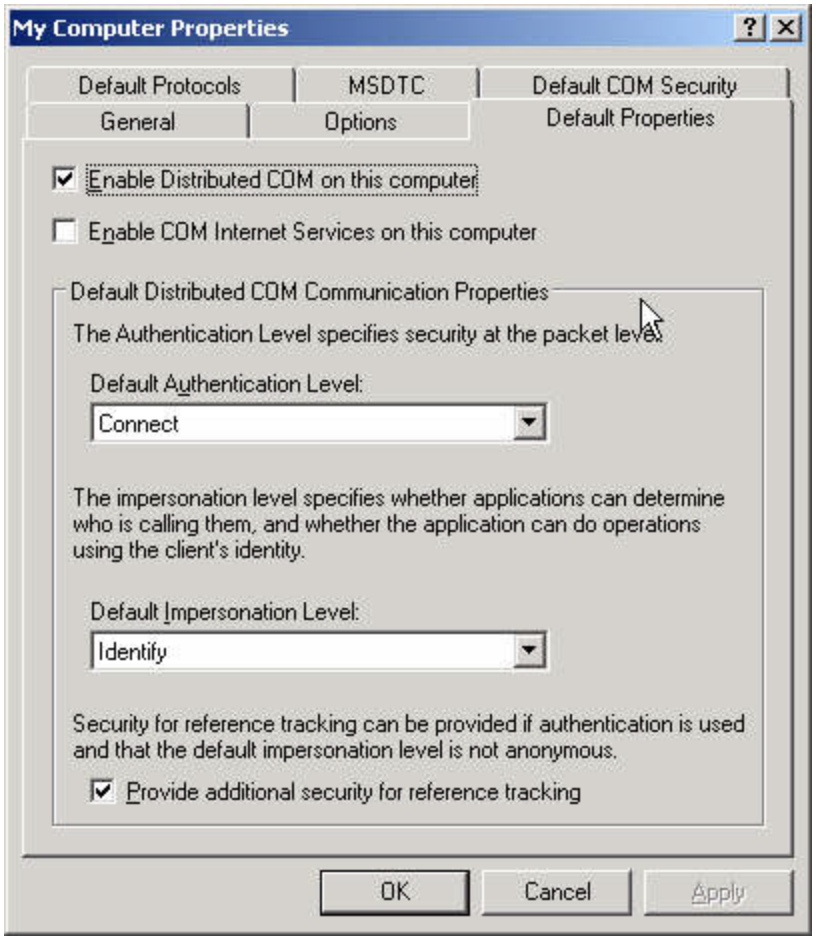
Default Properties

Default COM Security

MSDTC

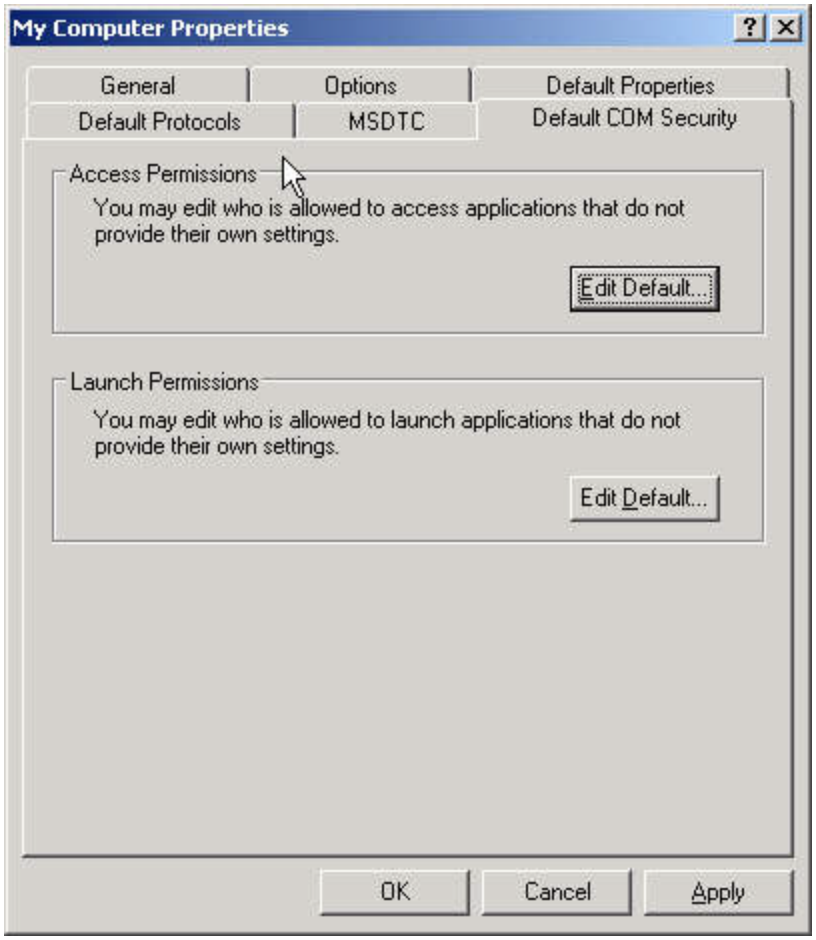
Default Protocols

Select the **Default Properties** tab. The following screen is displayed:


My Computer Properties
Default Protocols
MSDTC
Default COM Security
General
Options
Default Properties
Enable Distributed COM on this computer
Enable COM Internet Services on this computer
Default Distributed COM Communication Properties
The Authentication Level specifies security at the packet level.
Default Authentication Level:
Connect
The impersonation level specifies whether applications can determine who is calling them, and whether the application can do operations using the client's identity.
Default Impersonation Level:
Identify
Security for reference tracking can be provided if authentication is used and that the default impersonation level is not anonymous.
Provide additional security for reference tracking
OK
Cancel
Apply

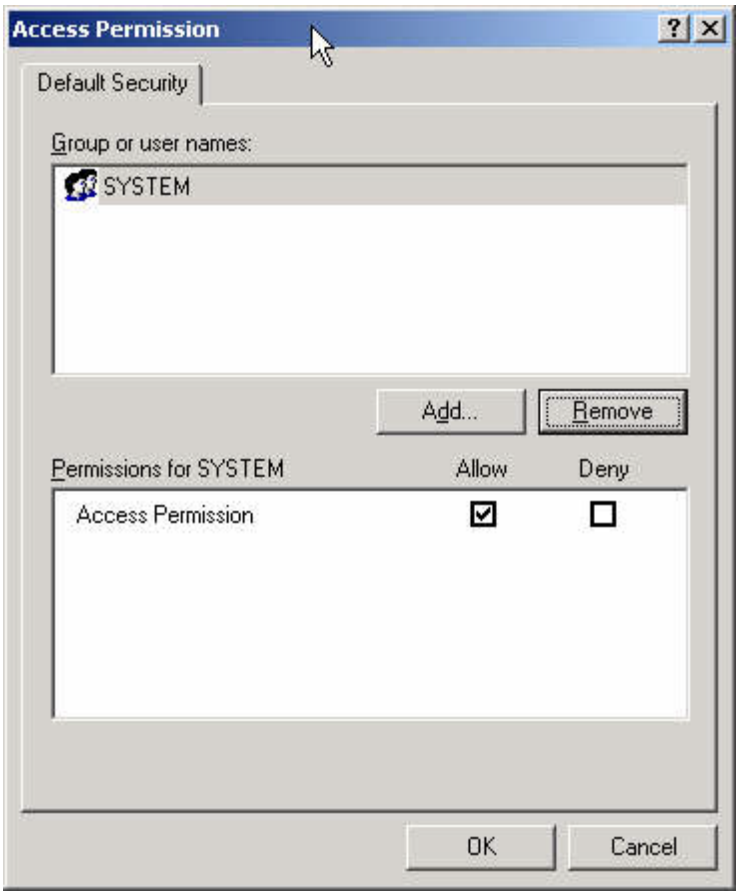
Make sure that the check box Provide additional security for reference tracking is checked.

Select the **Default COM Security** tab. The following screen is displayed:

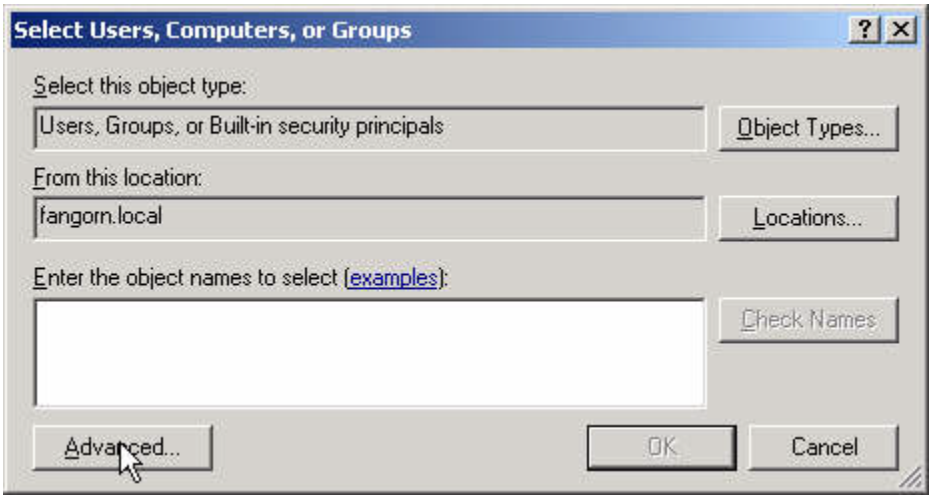


For the Access permission:

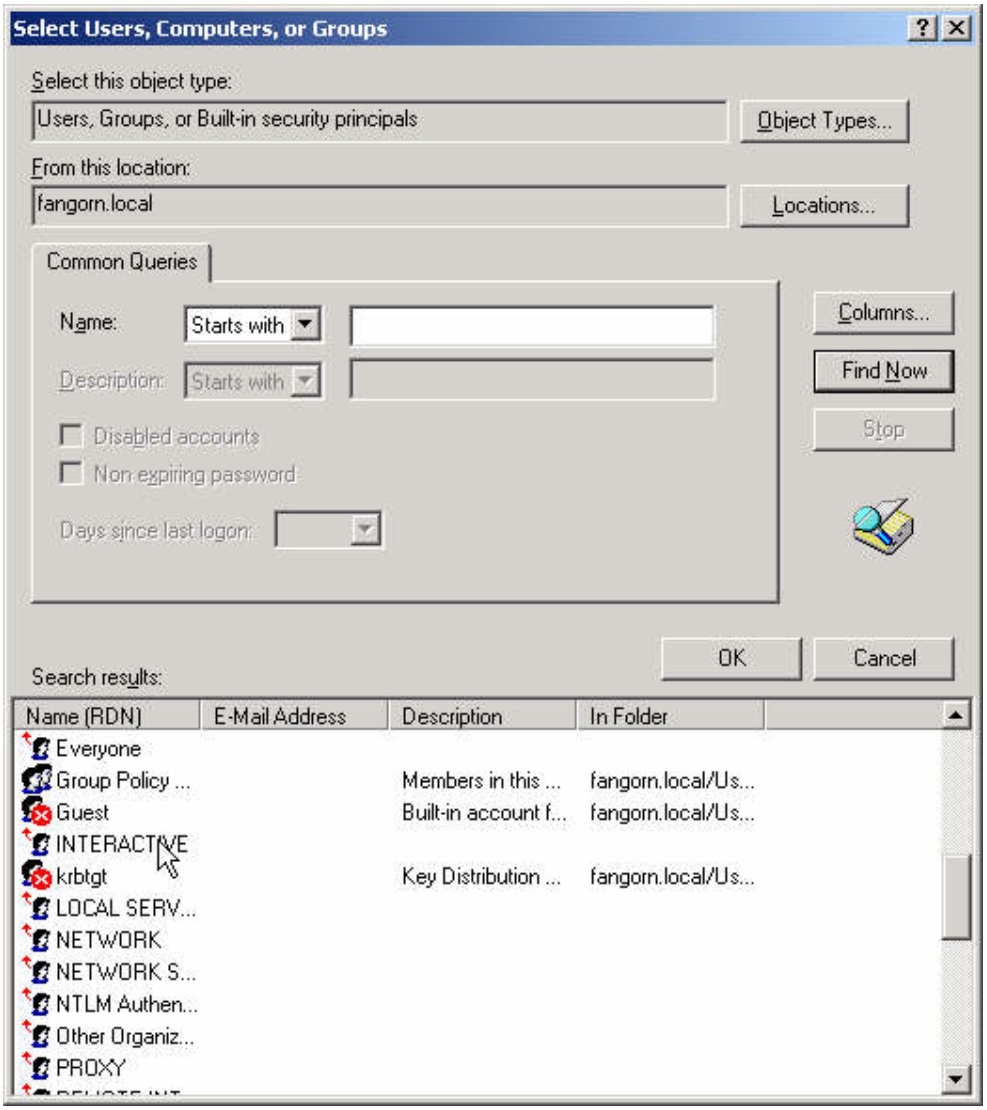
Click on the *Edit Default* button, to access the configuration windows (see below).



Click then on the *Add* button, the following window is displayed.

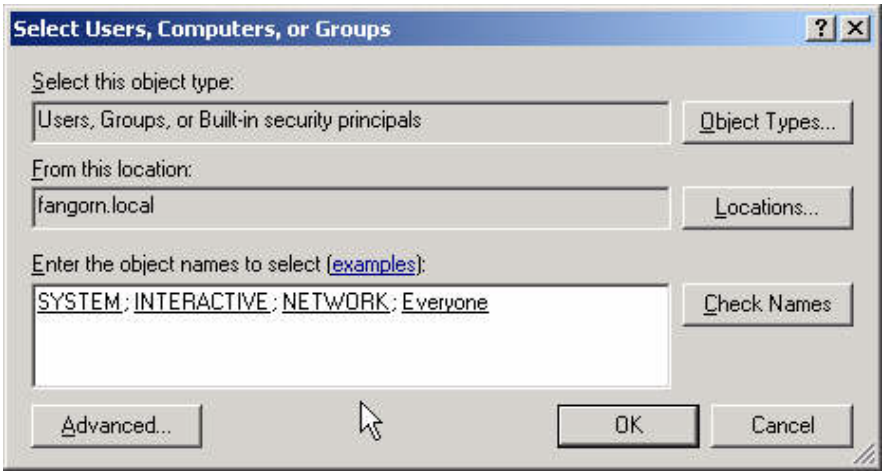


Click then on Advanced, the following window will then be displayed.

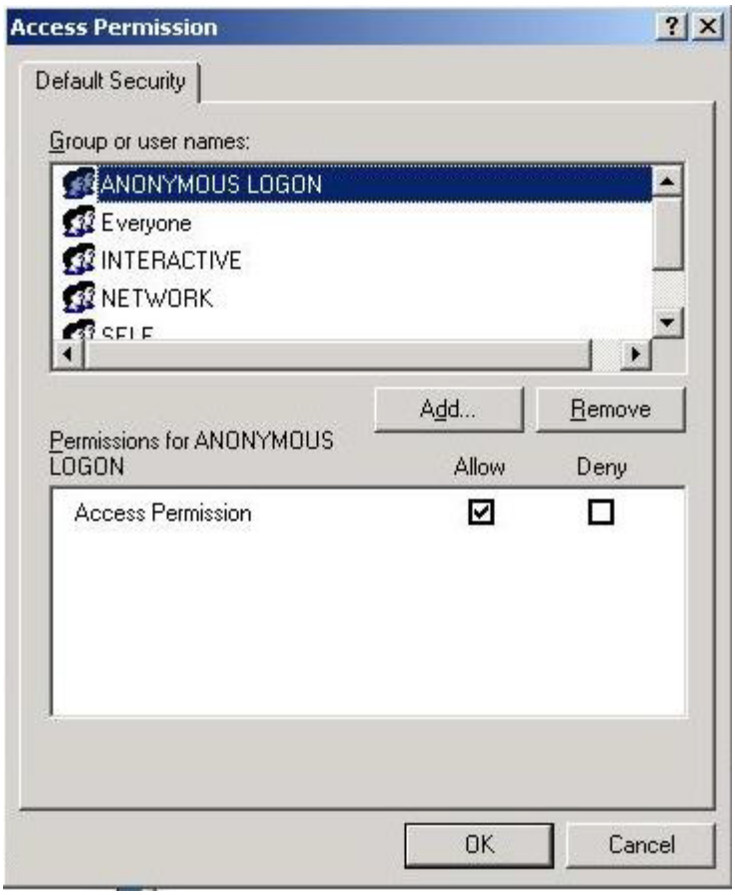


Select INTERACTIVE and press OK. Repeat the steps 3 to 5 to add *NETWORK; SYSTEM; EVERYONE.*

The following screen should then be displayed.



Click on *OK* and the Access Permissions should be configured as shown below.



Default Access permissions:

INTERACTIVE Allow Access

NETWORK Allow Access

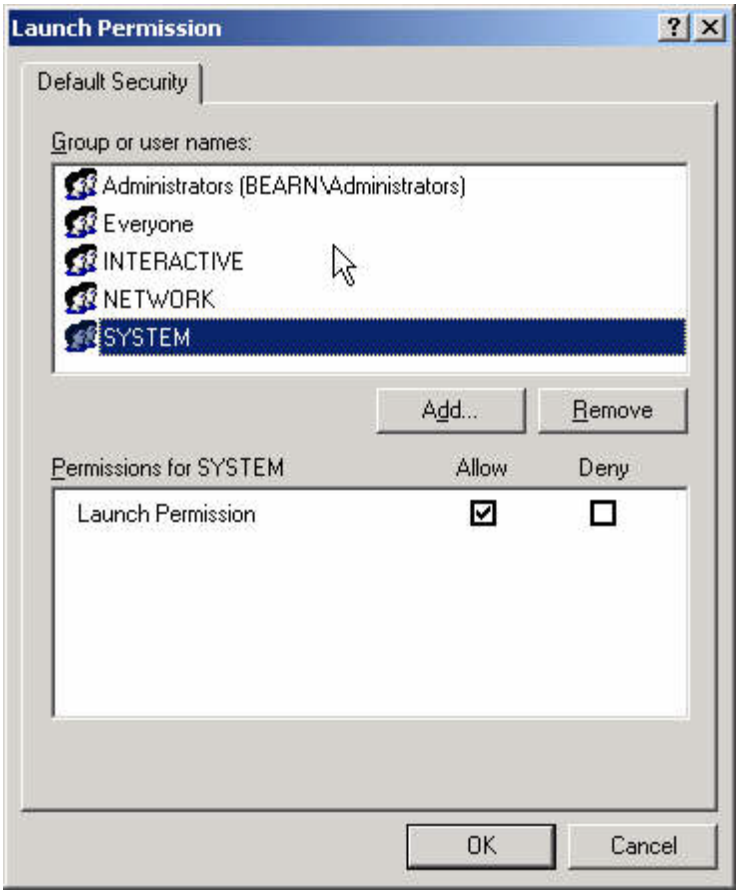
SYSTEM Allow Access

Everyone Allow Access

Anonymous LOGON Allow Access

For the Launch permission, do the same as for the Access Permission without the Anonymous Logon permission.

The Launch permission should be set as below.



Default Launch Permissions:

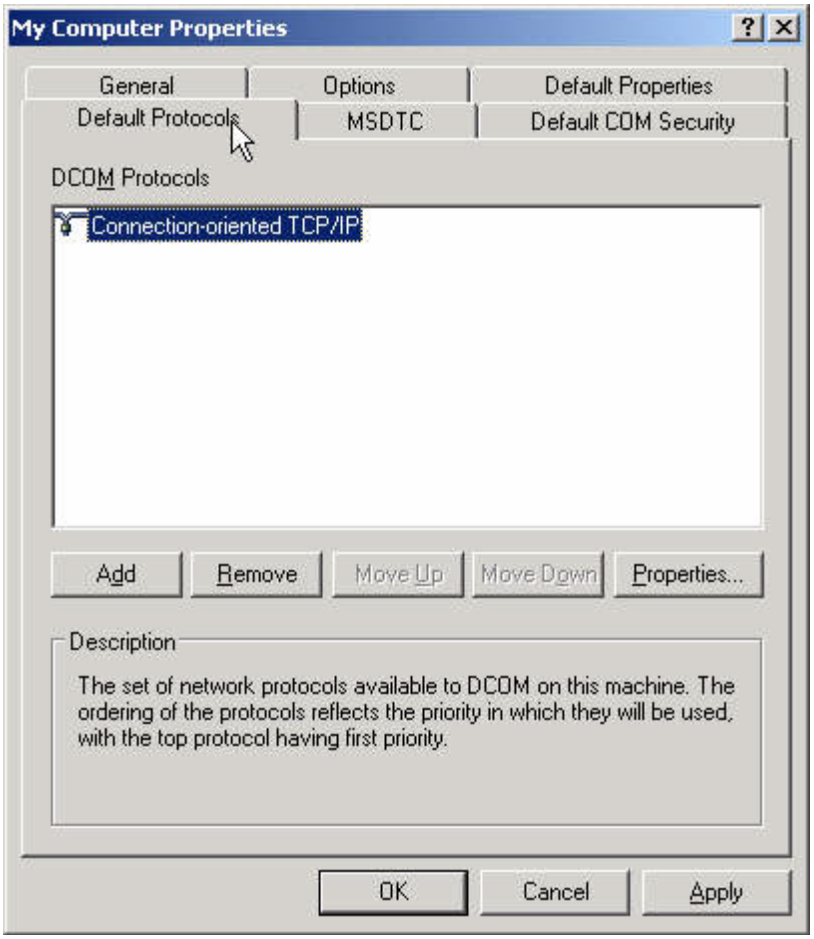
INTERACTIVE Allow Launch

NETWORK Allow Launch

SYSTEM Allow Launch

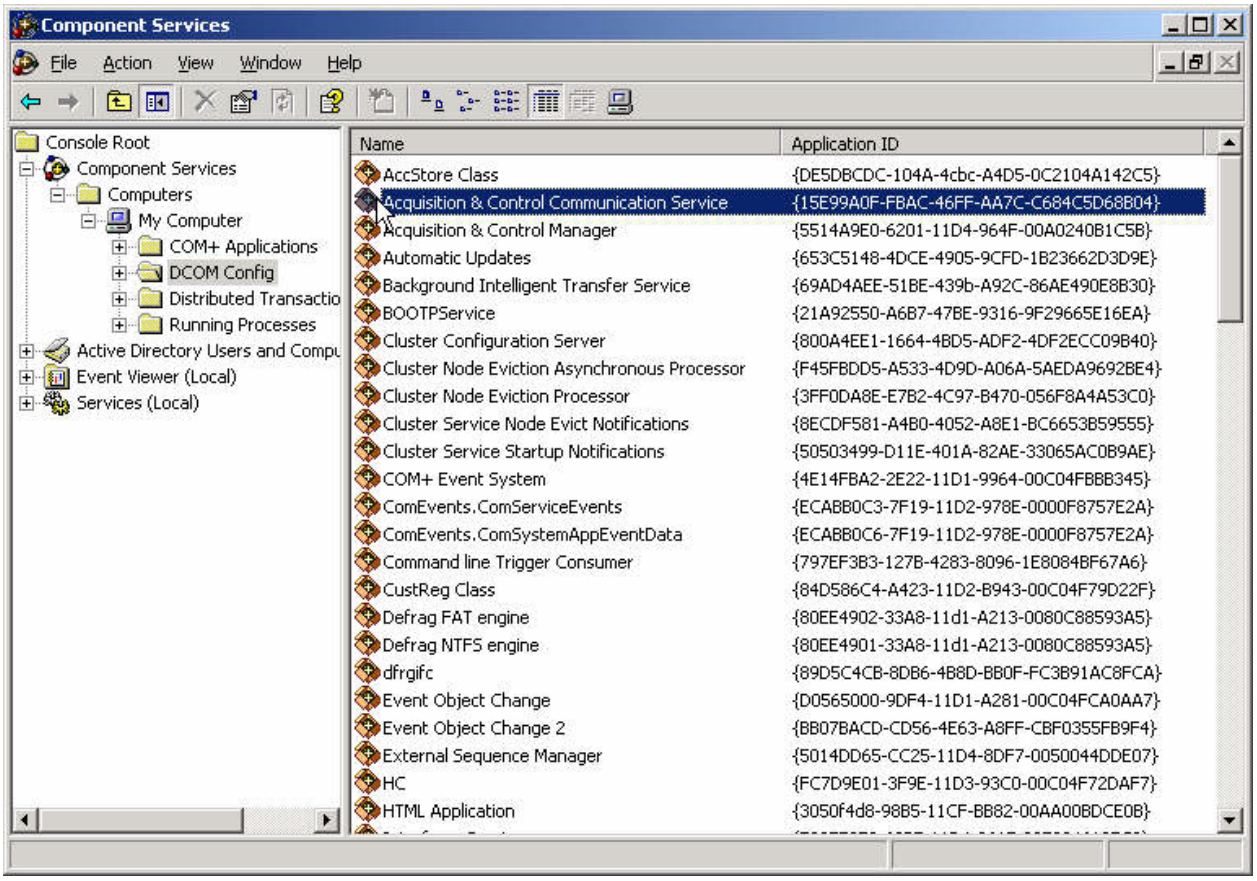
Everyone Allow Launch

Select the Default Protocols tab:



Select Connection-oriented TCP/IP and define it in the first position using the *Move up* button.

Close the Computer Properties and select *DCOM config* as in the following window.



For each of the following applications, configure the appropriate Permissions:

Acquisition & Control Communication Service

Acquisition & Control Manager

External Sequence manager

Interface Service

Quick Start Engine

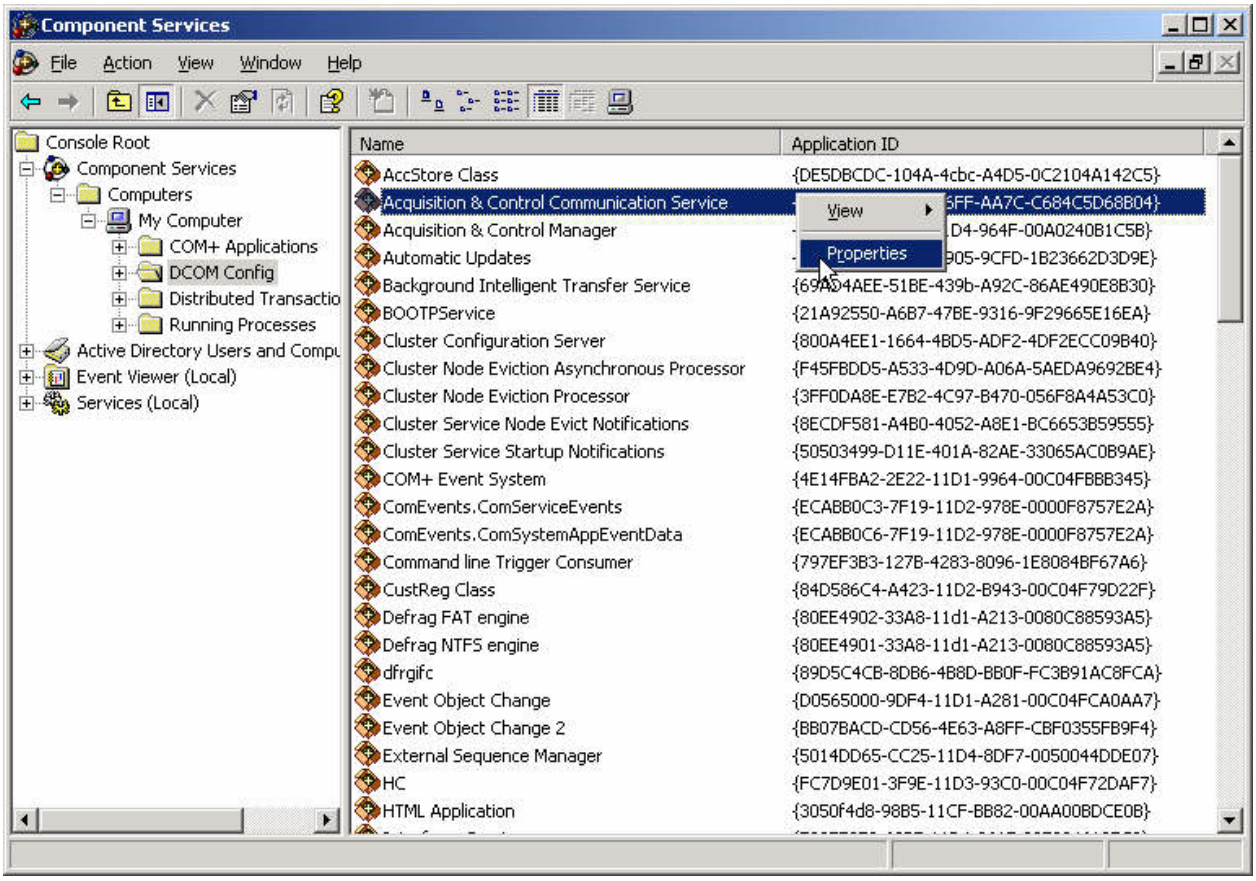
Quick Start Manager

Sequenceauto object or {38425FD5-F403-11D3-9246-0050044DDE07}

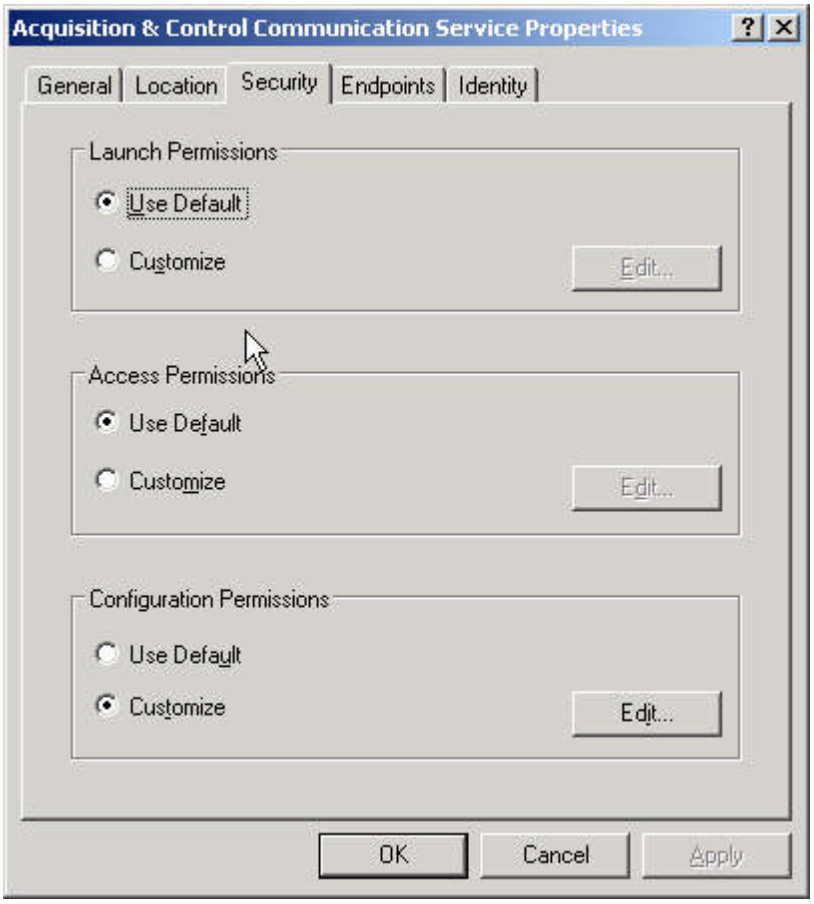
W2AutomationEngine object or {F1F76A40-9B57-49DCB7E2-92AF5039F4AC}

AcqManDiamirSide object or {4CDCE86D-C1CC-11D2-BEBD-00A0247B21AC}

Select each application properties with a right click as shown below.



In the opened window select the ***Security*** tab and select the *Default Permissions* for the first two types of permissions (Access and Launch).



Click on the *Apply* button to apply the modifications for each application.

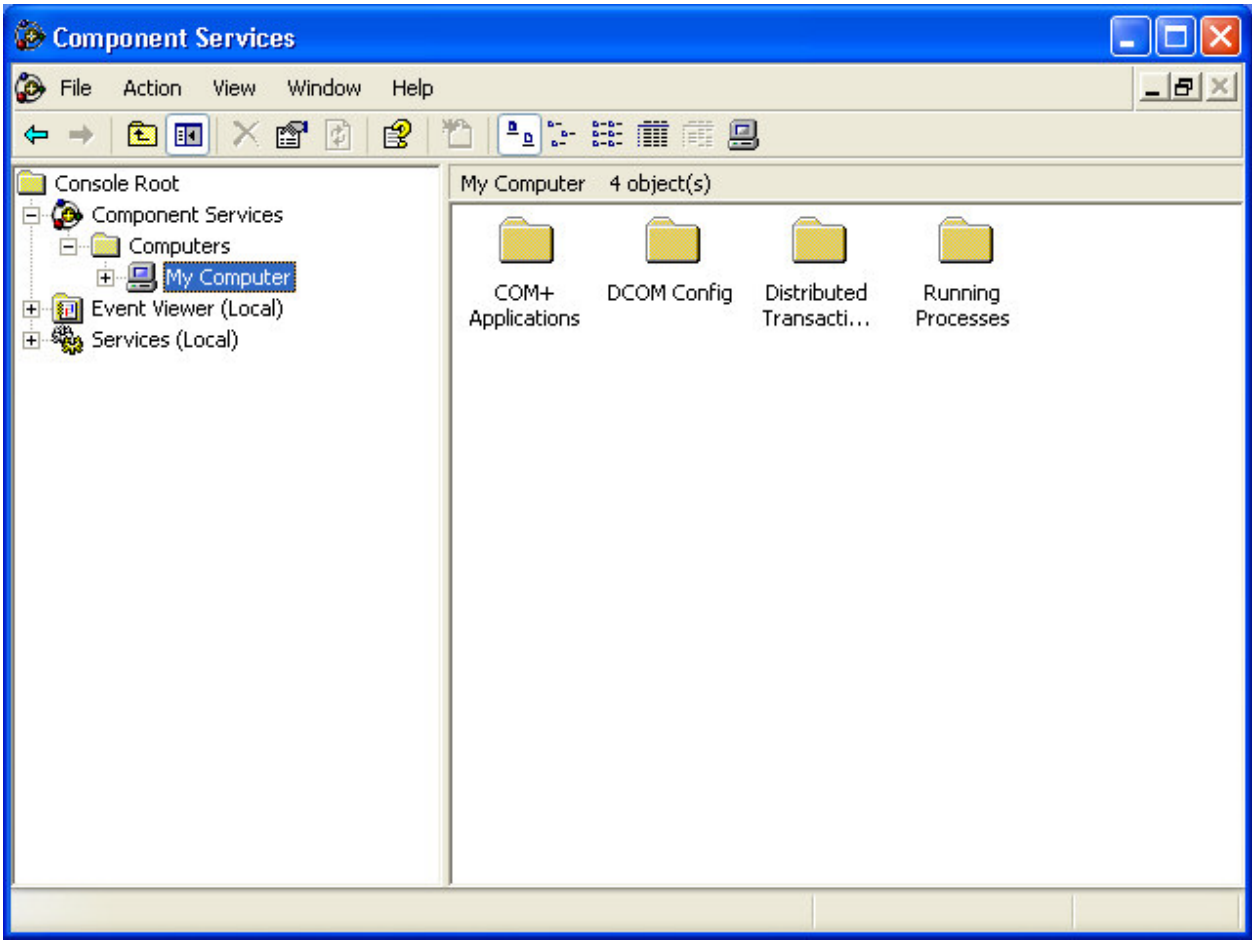
DCOM Configuration Under Windows XP SP2, Windows 2003

Server SP1 and Windows Vista (Enterprise & Business)

Please find below the procedure to configure DCOM under Windows XP SP2, Windows 2003 Server SP1 and Windows Vista.

Screenshots are made under Windows XP SP2 but they are the same under 2003 server SP1.

Connect under the Windows session as a local administrator in the ***START*** menu, in the ***RUN*** part enter ***DCOMCNFG***. The following window is opened:



1. Right click on *My Computer* and select Properties. A window is opened with 6 tabs:

   General

   Options

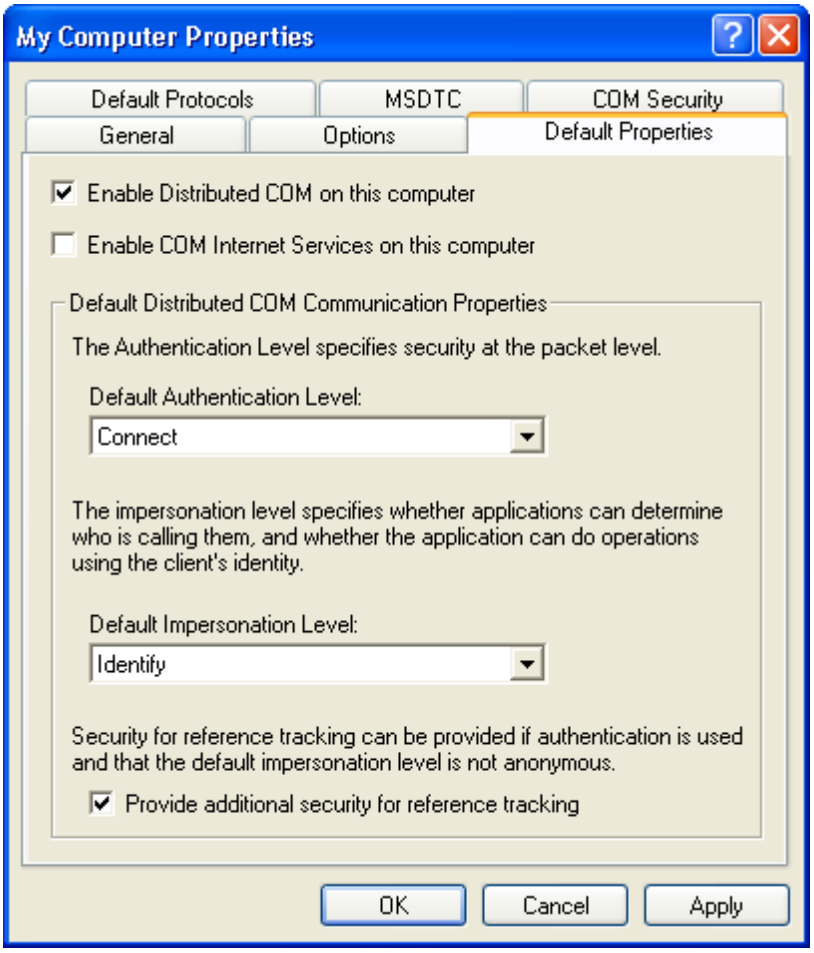
   Default Properties

   Default COM Security

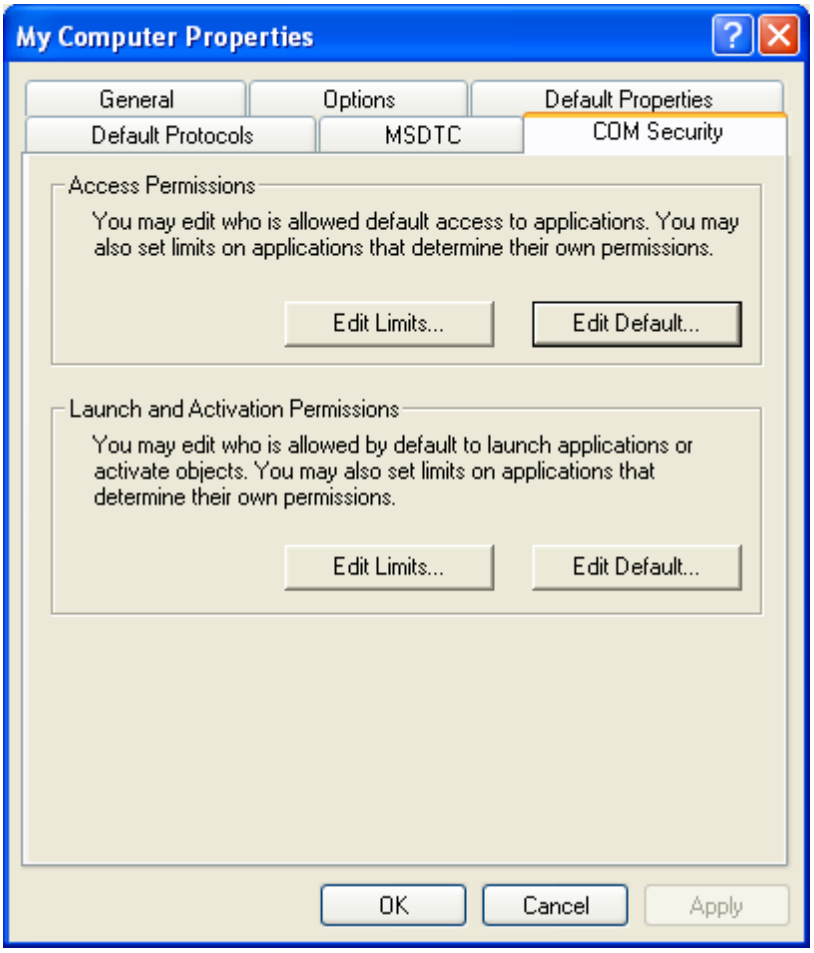
   MSDTC

   Default Protocols

Select the **Default Properties** tab. The following screen is displayed:

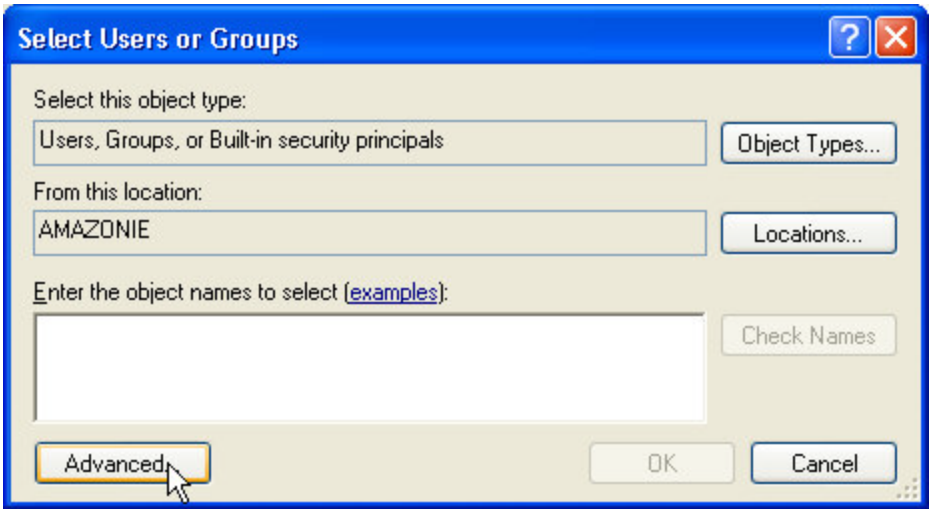

My Computer Properties
Default Protocols
MSDTC
COM Security
General
Options
Default Properties
Enable Distributed COM on this computer
Enable COM Internet Services on this computer
Default Distributed COM Communication Properties
The Authentication Level specifies security at the packet level.
Default Authentication Level:
Connect
The impersonation level specifies whether applications can determine who is calling them, and whether the application can do operations using the client's identity.
Default Impersonation Level:
Identify
Security for reference tracking can be provided if authentication is used and that the default impersonation level is not anonymous.
Provide additional security for reference tracking
OK
Cancel
Apply

Verify that *Enable Distributed COM on this computer* and *Provide additional security for reference tracking* boxes are checked. Select the **Default COM Security** tab. The following screen is displayed:

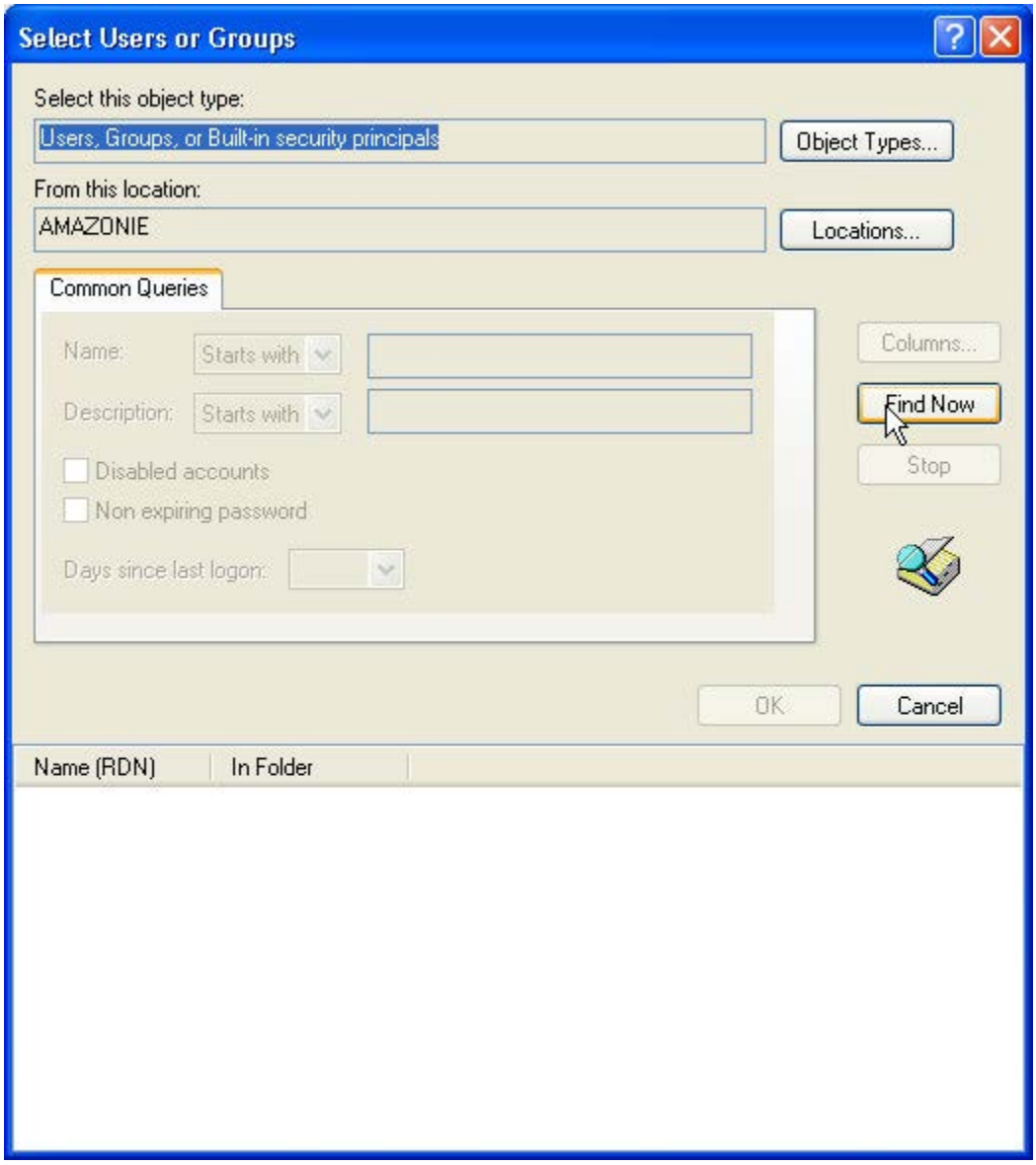

My Computer Properties
General
Options
Default Properties
Default Protocols
MSDTC
COM Security
Access Permissions
You may edit who is allowed default access to applications. You may also set limits on applications that determine their own permissions.
Edit Limits...
Edit Default...
Launch and Activation Permissions
You may edit who is allowed by default to launch applications or activate objects. You may also set limits on applications that determine their own permissions.
Edit Limits...
Edit Default...
OK
Cancel
Apply

For the Default Access permission,

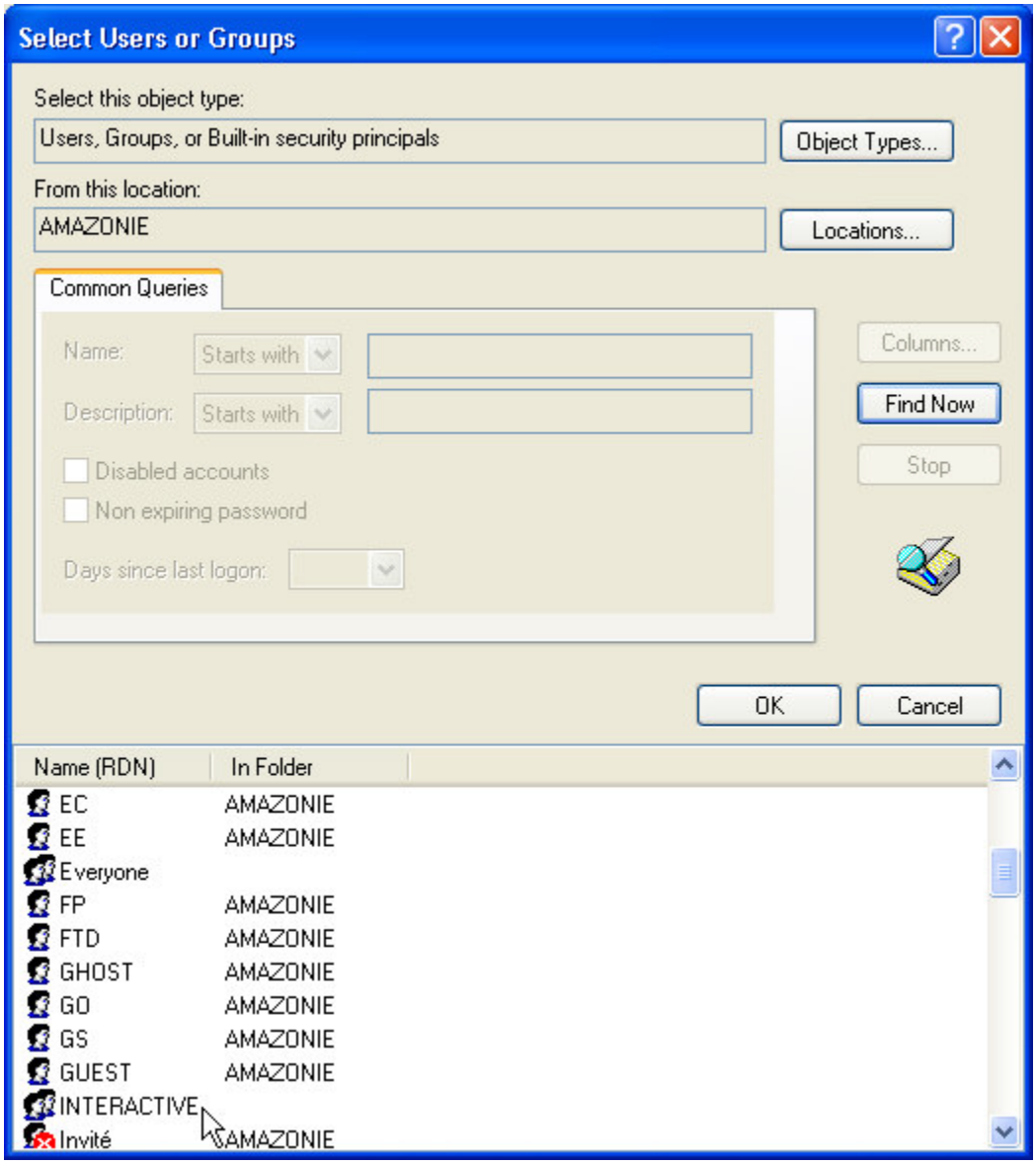
2. Click on the *Edit Default* button, to access the configuration windows.
3. Click then on the *Add* button, the following window is displayed.



4. Click on *Advanced,* the following window will be displayed.

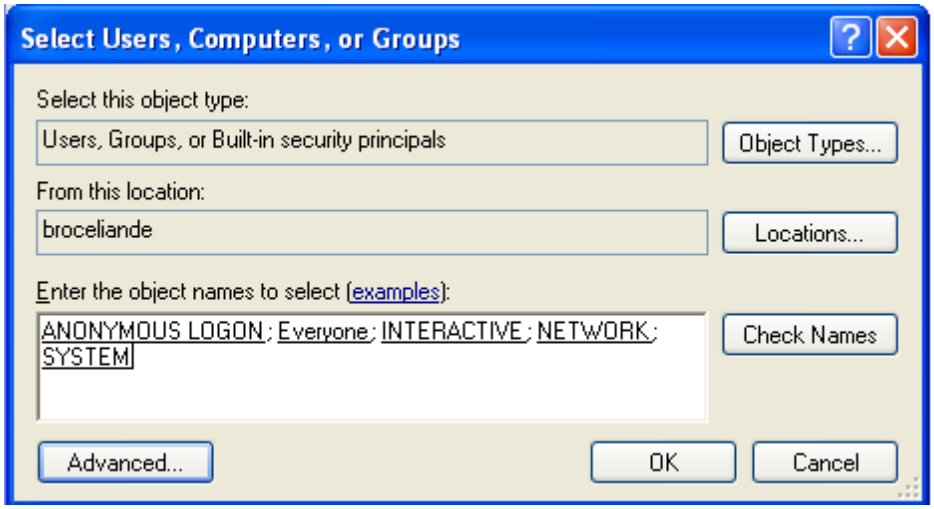


5. Click on the *Find Now* button to display the available permissions.

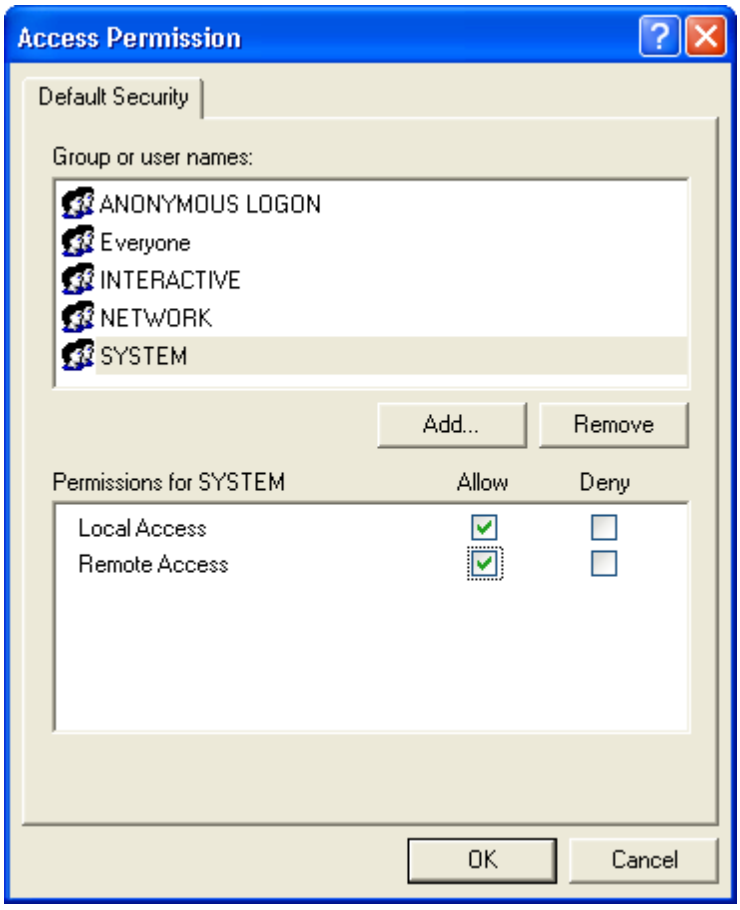


Select INTERACTIVE and press OK.

Repeat the steps 3 to 5 to add *NETWORK; SYSTEM; EVERYONE, ANONYMOUS LOGON.* The following screen should then be displayed.



Click on *OK* and the Access Permissions should be configured as below.



Default Access permissions:

• ANONYMOUS LOGON Allow Local Access

Allow Remote Access

• INTERACTIVE Allow Local Access

Allow Remote Access

• NETWORK Allow Local Access

Allow Remote Access

• SYSTEM Allow Local Access

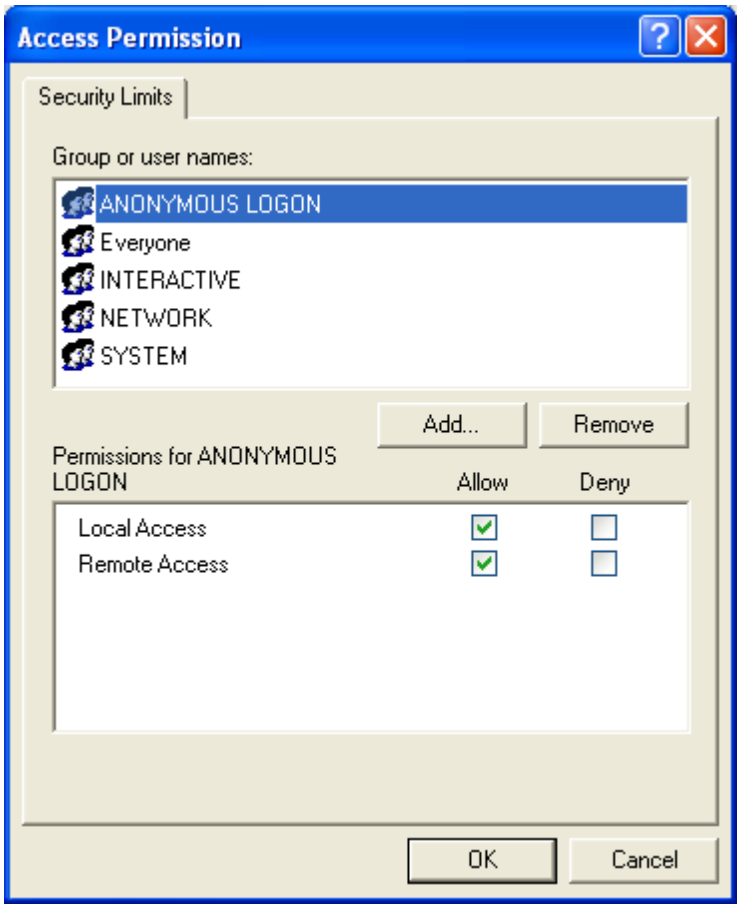
Allow Remote Access

• Everyone Allow Local Access

Allow Remote Access

For the Limits Access permission, do the same as for the Default Access Permission.

The Limits Access permission should be set as shown below.



CompassCDS
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501481
Revision D

Contents

Introduction 3
Software Presentation 3
Getting Started 4
Connection 4
Starting an Acquisition 4
How to View an Acquisition 8
Reprocessing a Chromatogram 11
Starting a Sequence 14
Application Details 16
Software Structure 16
The Method 38
CompassCDS Variables 110
Baseline Monitoring / Quick Start / Sequence 139
The Calibration Curves 160
Manual Integration and Identification 170
Reprocessing a Chromatogram 173
Viewing the Results 180
Integration Results Display on the Chromatogram 180
Summary Report 194
Importing a Chromatogram (AIA format) 204
Audit Trail 204
How to Compare Two Chromatograms 207
Electronic Signature 208
Lock/Unlock Chromatograms 222
Advanced Parameters 225
IntelliUpdate 225
Remote Sequence 227
Retention Index 232
CompassCDS ASCII Import 240
CompassCDS Print manager (PDF Export) 240
CompassCDS Arithmetic functions 240
Procedures 241
How to Acquire a Chromatogram 241
How to Define a Sequence for Analysis Execution 244
How to Build a Process Method 245
How to Reprocess a Chromatogram 247
How to Build a Calibration Curve 249
How to Print a Customized Report 250
How to Print a Calibration Curve 252
Glossary 253

Introduction

Software Presentation

CompassCDS is a state-of-the-art, chromatography software platform that provides a choice of complete pull-down task menus, user-friendly icons, and easily accessible popup menus within specific windows. The browser and task wizards enable new users to quickly complete their tasks, making CompassCDS a very “easy to learn” chromatography software.

CompassCDS can acquire data from GC systems. The control methods for such instruments are fully integrated within the CompassCDS interface.

CompassCDS is able to effectively integrate most chromatograms automatically using only two parameters: peak width and noise threshold which are entered at time zero. These parameters are automatically updated and the system applies the optimum values for each chromatogram. In some cases specific integration events may be required to integrate complex chromatograms. These are readily available within CompassCDS. Reference peaks may also be used for peak identification, and several calibration modes are available including normalization, external or internal standard, with response factors or calibration curves. CompassCDS can also quantify peaks within a group using a common response factor or calibration curve.

CompassCDS enables users to define custom variables via a unique variable editor and to also summarize reports with control charts and tables which can be built to monitor the evolution of analysis results. System suitability tests can also be performed automatically on all CompassCDS variables, including user-defined custom variables.

Customized analysis reports can be configured within CompassCDS Report Editor, the CompassCDS custom report editor. Chromatograms, results tables, calibration reports, etc. with customized formatting and presentation can be inserted and then saved as a report style file. Report styles can be recalled later or edited and saved as another report style file.

The use of the individual instrument control drivers, CompassCDS Configuration Manager, CompassCDS Report Editor, the report builder, and all optional processing modules are explained in detail in separate user guides that are provided with the corresponding applications.

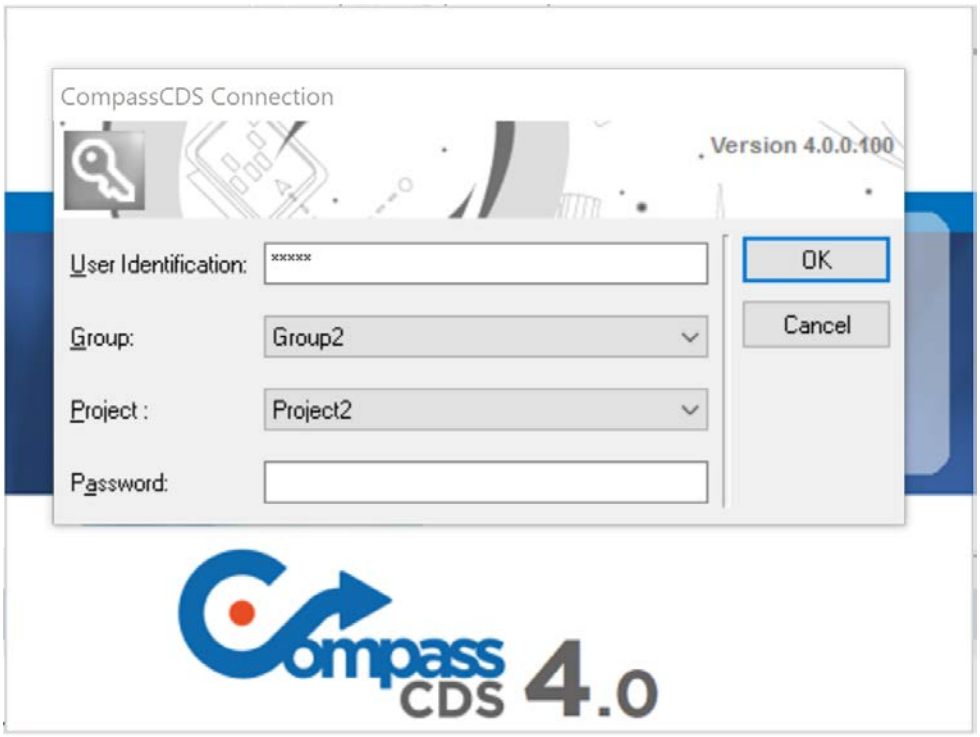
How to use this manual when using CompassCDS for the first time

Start by reading the "Getting Started" section. This section contains essential information about acquisition and chromatogram handling. More detailed information for each individual function can be found in the section “Application details.”

Getting Started

Connection

If the default domain is defined during the installation, the following logon box is displayed when starting CompassCDS:



The user must enter their ‘User identification’, and choose in the scroll box the group and the project in which to work and, if necessary, type in a password. The password is case sensitive, meaning that abc is different from ABC. User names and passwords will be assigned by the system administrator or can be set by logging into the CompassCDS Configuration Manager application, using an administrator login, and creating/editing a user.

When a user connects for the first time, the user will be asked to change the password.

Starting an Acquisition

The first step is the creation of a method, which then enables the acquisition of chromatograms. This method will be associated with the chromatogram once the data has been acquired.

Creating the Method

From the menu, select FILE / NEW / NEW METHOD.

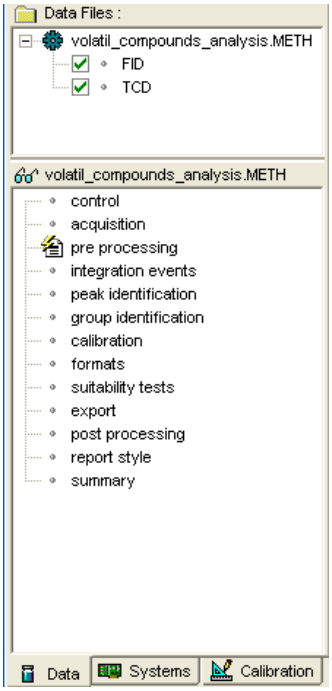
Select the project in which the method will be used (when in all projects mode) and the chromatographic system, to which the method will be applied.

Click Next.

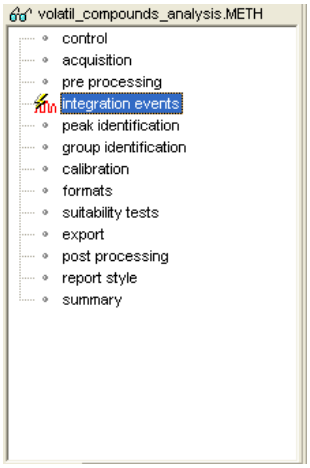
Enter the name of the method, and a method description (optional) which will appear as a comment in the Open File window. The un-edited method is opened with default settings and parameters listed in each section of the method tree.

To display the different sections of a method (acquisition parameters, integration parameters, etc.), click on the corresponding item in the method tree. Methods created for multi-channel instruments will show both channels in the top section of the browser as shown below. To select a channel, a user clicks on that channel and the method tree corresponding to that channel will appear in the browser.

To select the FID channel …



To select a method section in the method tree…



Defining Method Parameters

In the method tree in the browser, clicking on the control section displays the parts of a method associated with instrument control.

If the instrument is being fully controlled by CompassCDS, a user can enter the required instrument control method parameters.

In the method tree in the browser, clicking on the acquisition section displays the fields associated with each injection such as Run Name, Run Time, Injection volume.

Parameters set in this section will appear by default in the acquisition start windows (Quick Start and sequence). For example, the run name can be entered (the identifier or suffix will be implemented automatically for each run in the case of a Quick Start) and the run length.

NOTE: In the chromatograms acquired, the parameters of this field will be the ones entered for the acquisition. If a reprocess of the acquired chromatogram is done, the acquisition parameters will not change in this field.

In the method tree in the browser, clicking on the Integration section displays the fields associated with integrating chromatograms.

This section enables a user to set the integration parameters required for the correct integration of chromatograms. In the case of simple chromatograms, the two default parameter settings should be sufficient to integrate the chromatogram. Entering the approximate width of the peak of interest in the peak width parameter box, and a value for the 'threshold' to define the start and the end of a peak, according to the slope of the signal and then re-integrating (F5) enables users to optimize the integration parameter settings for specific analyses

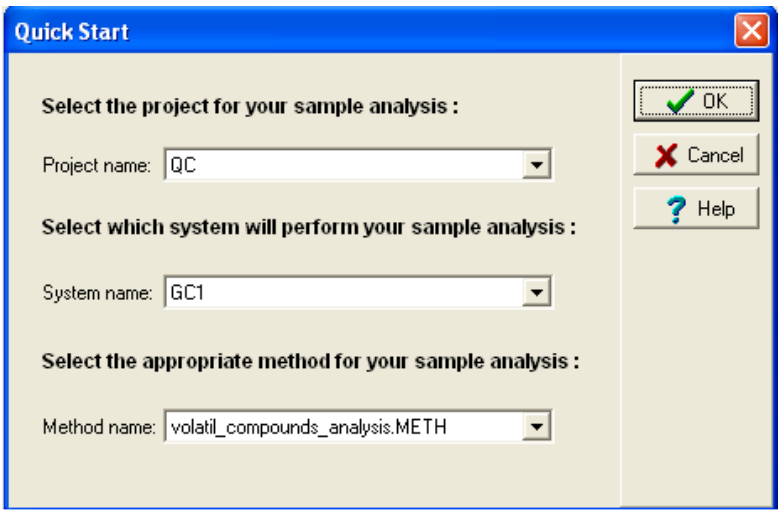
These parameters are all that are required to start an acquisition. Other method parameters, e.g., “Peak Identification”, “Calibration” or “Grouping”, can be selected later once example data for the application exists.

Save the method by using the pull-down menu selection

FILE / SAVE / SAVE METHOD, clicking on the Save Method icon or by pressing the key combination Shift+Ctrl+2.

Starting an Acquisition

Selecting ACQUISITION / QUICK START from the pull-down menu brings up the Quick Start window.


Quick Start
Select the project for your sample analysis :
Project name: QC
Select which system will perform your sample analysis :
System name: GC1
Select the appropriate method for your sample analysis :
Method name: volatil_compounds_analysis.METH
OK
Cancel
Help

The three fields in this window are filled in by either typing names or selecting these from the drop-down lists:

- The project (if connecting into CompassCDS in all projects). If the all projects option is not selected for a user (default state) then only the following two fields are displayed.
- The chromatographic system or instrument on which sample is to be analyzed.
- The name of the analysis method.

Clicking on OK displays a window for entering or confirming the acquisition parameters.

The following minimum set of parameters must be entered:

- The chromatogram name (File Name and Run identifier that will be used to create the name).
- The acquisition run time in minutes.

If a CompassCDS controlled system is configured with a fully controlled autosampler the following additional information must be entered:

- The injection volume.
- The vial number in the tray and, if necessary, the rack number.

Pressing Start once the acquisition parameters have been entered will start an acquisition.

If the system is not using an autosampler, the sample can be manually injected and pressing start on the chromatograph will initiate acquisition.

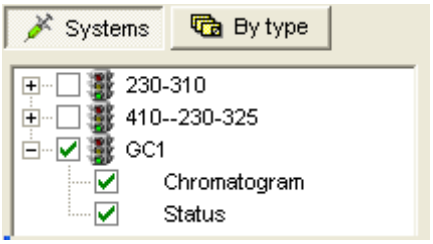
How to View an Acquisition

Viewing an Acquisition

From the CompassCDS main screen, click on the Systems tab (bottom left of window) to go to the Systems view.

In the browser, a user then selects the system into which the sample was injected by checking the appropriate checkbox. Clicking the chromatogram checkbox enables users to view the data acquisition. Clicking the status checkbox enables users to also view the system status.

NOTE: The ✔ symbol in front of the system name indicates that the system is selected. By default, both 'chromatogram' and 'status' are selected when the system checkbox is selected.



An idle system is preceded by the symbol, while a system which is busy downloading a method or waiting for an injection in preceded by , and a running system is preceded by .

The chromatogram(s) is displayed and refreshed automatically throughout the entire acquisition.

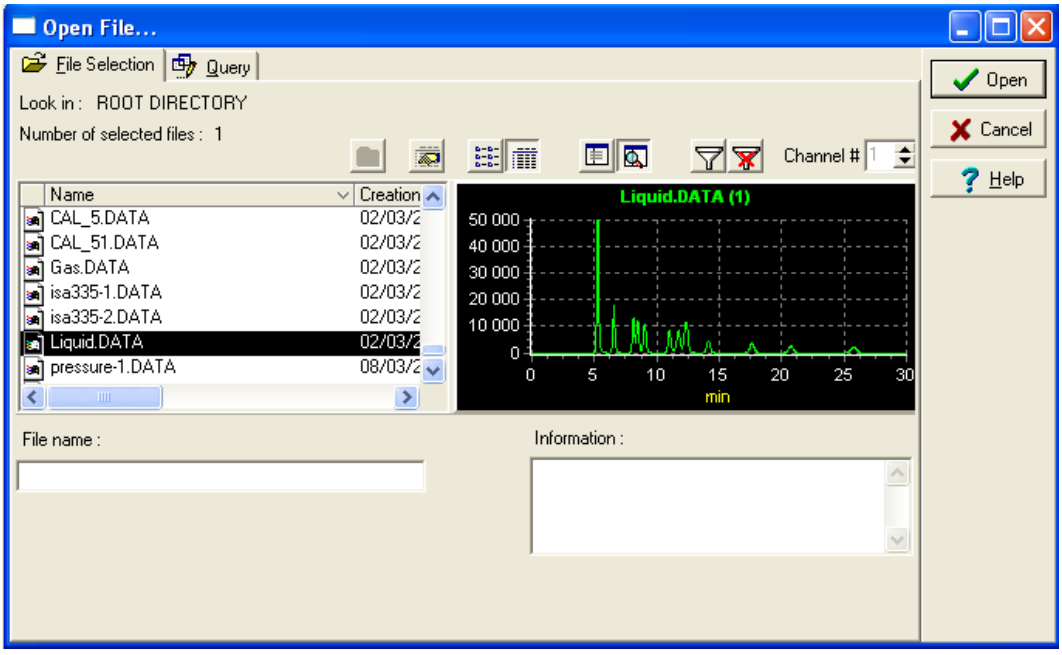
In order to stop an acquisition before the end of a run, a user can press the *Stop* button . If the chromatographic system is not fully controlled (e.g.,, data acquisition only), the data acquisition process will be terminated. If the system is fully controlled, the button will stop either only acquisition or acquisition and the chromatographic system according to the driver configuration.

In this case, the chromatograph remains active, e.g., in the case of a GC, although data acquisition has stopped, the oven temperature program will continue and the chromatograph may have to be stopped manually.

Viewing a Chromatogram

Once the chromatogram has been acquired, it can be opened and processed:

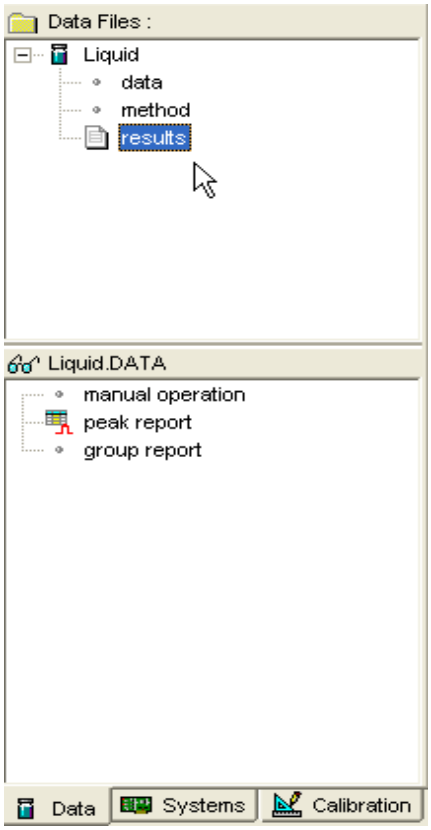
Selecting FILE / OPEN / OPEN CHROMATOGRAM or pressing causes the Open File window to appear:



In this window, users can use the scroll bars to scroll down the list and click on the most recently acquired chromatogram. Alternatively, typing the first few letters of the chromatogram name in the file name box will display only the chromatograms with names beginning with these letters. Clicking on the Open button or double clicking on the selected chromatogram will cause it to be displayed in the Data view.

The selected chromatogram, which will have already been processed and the results table, will be displayed on the screen.

In the browser, click on Results to view the integration results table.

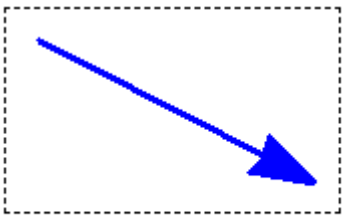


Clicking on Peak report enables users to view the results calculations for each peak.

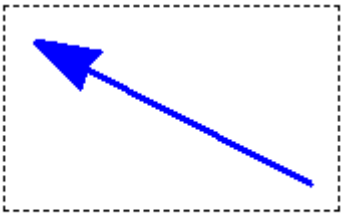
The peak report is displayed in the right panel below the chromatogram.

The results (peak names, baseline, and integration marker) are also displayed on the chromatogram.

Users can zoom in or out of a displayed chromatogram by clicking and dragging the left mouse button. Top left to the bottom right of the screen will zoom in and bottom left to top right will un-zoom.

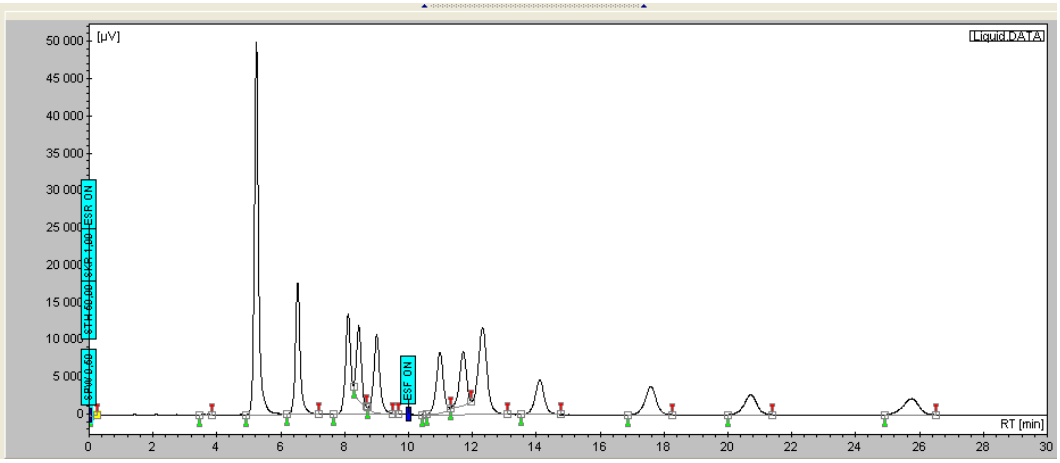


Zoom in



Zoom out

Clicking on the bar directly a displayed chromatogram will display or hide the chromatogram.



Reprocessing a Chromatogram

Once the chromatogram is opened, it is possible to modify the chromatogram results. This may be done either by modifying the method associated with the chromatogram or by modifying the integration or the identification manually.

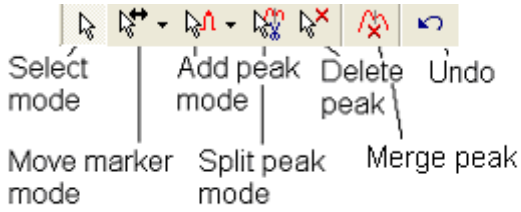
Integration

In automatic mode:

Change the integration events in the corresponding section of the method, and press F5 or click on the *Calculate* icon to view the changes.

In manual mode:

Use the manual integration bar to manually modify the integration.



In Select mode, click on a marker to select the corresponding peak, then select the icon corresponding to the desired action.

In Move marker mode, click on the marker to move, and then click on the new marker location.

In Add peak mode, click where the peak should start, then click where the peak should stop.

In Split peak mode, click on the place the peak should be split.

In Delete peak mode, the currently selected peak is deleted. THEREFORE, MAKE THE PEAK SELECTION BEFORE CLICKING ON THE DELETE PEAK ICON. (The selected peak markers and report line are highlighted in yellow).

In Merge peak mode, the currently selected peak is deleted and the next peak is extended to the left in order to include the deleted peak. This option is available only if peaks are separated by a valley or have been split.

Each time the integration events are modified manually, the modification action is saved within the Manual operation and can be removed using the Undo icon . Click on Results/Manual integration in the browser to view the manual modifications.

Identification

In automatic mode:

Change the identification table and press F5 or the Integrate icon to view the changes.

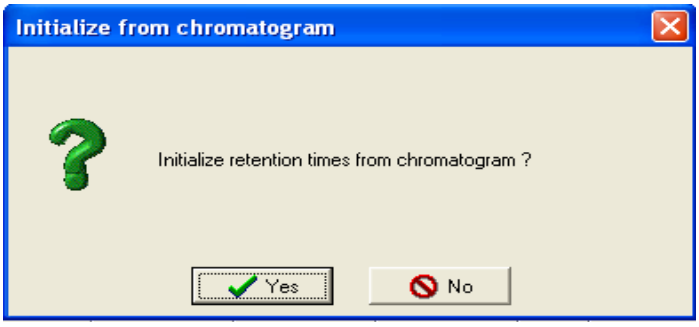
In manual mode:

Display the result table (click on Results/Peak report in the browser), then edit the peak names in the table. Double-click in the 'Name' column and type the new name to rename the peak manually.

As with manual integration, this operation is saved in the Manual events and can be removed with the Undo icon .

If the identification is not correct, it is possible to rename the peaks manually and then update the changes in the identification method:

Select Method and then Identification in the browser. To update the retention windows, press the right mouse button in the identification table and select Initialize retention times from chromatogram. Answer yes to the confirmation message:



Reprocessing

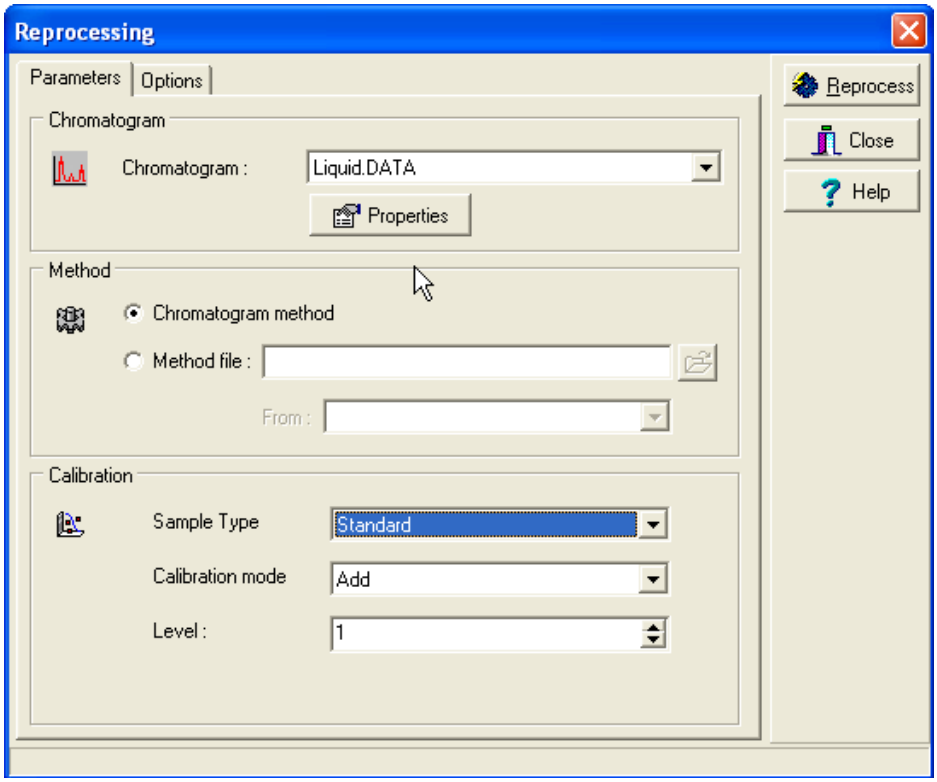
If the Identification section, Integration section, or the Variables are changed, press *F5* or click on the *Integrate* icon to view the changes.

If the Export, Post Processing, Print report or Summary sections are changed, the chromatogram must be reprocessed.

If the Calibration section is changed, recalculating is sufficient only if the analysis performed is for an Unknown sample. However, if the sample is a Standard, then this sample must be reprocessed by clicking on the r*eprocess* icon or by pressing the F6 key.

To reprocess a chromatogram, select PROCESSING / REPROCESS.

The Reprocessing window appears:



In this window, select the name of the chromatogram to process from the list of all the open chromatogram names. The selected chromatogram is chosen by default.

Now select the method to be used to process the chromatogram. By default, the chromatogram will be processed with the method associated with it. If the chromatogram must be reprocessed with an external method, check the Method file option, and press to select the method name in the Open File window.

In the Calibration area, select Unknown if the chromatogram is an unknown sample or Standard Level X if the sample is a standard corresponding to the Level X in the Calibration method. In the case of a standard (the calibration section of the method has to be correctly completed first), check “Clear old points” to delete previous calibration points or check “Clear this level only” to delete the points corresponding to the same standard level. Do not check anything to add a point to an existing calibration curve.

By accessing the Option pages, it is possible to uncheck some of the processing features so that they will not be run during the processing. In the case of a two-channel method, the "Options" page is divided into 2 tabs (one for each channel). Thus, it is possible to perform some actions on one channel and others on the second one.

Once all the parameters are set, press the Reprocess button to start the reprocessing. A message in the status bar at the bottom of the screen indicates that the calculation is completed.

NOTE: If the chromatogram has been treated as a standard, a calibration curve is generated. To display this curve, select the menu FILE / OPEN / OPEN CALIBRATION CURVE, and select the name of the calibration curve. The corresponding curve(s) is/are displayed on the right page.

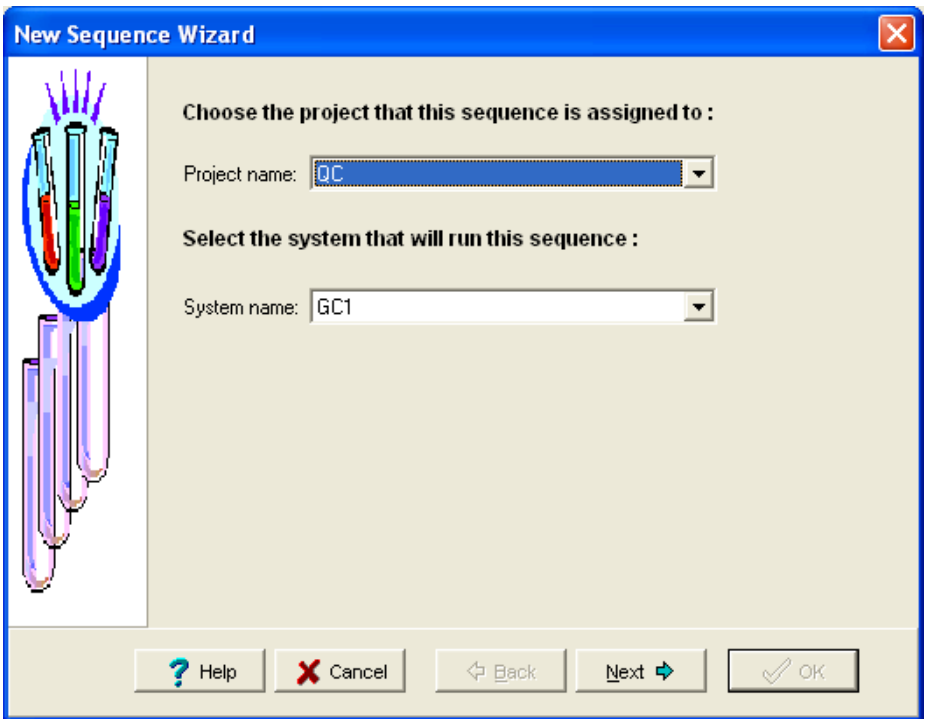
NOTE: If the properties of the chromatogram are modified, they will not be displayed in its acquisition part (which cannot be overwritten), but the new values will be visible in the variable part as global variables.

Starting a Sequence

To start several acquisitions at the same time, the corresponding processing methods need to be first created. It is then possible to create the sequence.

In the main menu, select FILE / NEW / NEW SEQUENCE:

A window appears for selecting which system is to be used to inject the samples:



Select the project (if connected in all projects) and the system and press Next, enter the number of lines (samples) for the sequence and press OK.

NOTE: Only one system can be used by sequence.

In the Browser, a new object is added corresponding to this sequence.

Click on the Icon '+' to add additional sample lines to the sequence table.

In each line of the sequence, enter the name of the method that will be used for acquisition, processing, and editing of the chromatogram.

Some cells of the line are filled automatically with the parameters entered in the acquisition part of the method.

The minimum parameters that must be entered are:

- The chromatogram name (File prefix and Run identifier that will be used to create the name).
- The acquisitions run time in minutes.
- The user input variables if some have been defined in the method with a mandatory feature.
- The istd values, if an internal standard calibration has been defined in the method.

If CompassCDS controls an autosampler:

- The injection volume.
- The vial number in the tray and, if necessary, the rack number.

To fill the cells quickly, use the ‘Fill block’ icon . (Or the fill block option in the popup menu), for example, fill-in the first RunID (suffix) cell, then select this cell with all the cells to be filled, and press the ‘Fill block’ icon .

A window called ‘Auto fill block’ appears.

Press OK.

The cells are filled with incremented integers or a copy of the first cell.

Save the sequence, and then launch the sequence with the Run icon .

Application Details

Software Structure

Logon

When initially starting the CompassCDS, a logon is required that will identify each person with a user name and the project(s) and group in which the work will be performed. This amounts to specifying a working directory, a profile, etc. The working directory is the directory where the data are stored, i.e., the file path when opening or saving a file. The profile is defined for a user or several users and specifies the rights to perform the various actions in CompassCDS. If a menu or a certain button is deactivated, the user does not have the access privilege or rights to perform the corresponding action. A prompt for password entry may also be required for certain tasks.

Users with the right to log on all projects will have the possibility to choose “All projects” as the project name. This enables them to view all files in all projects and to control all instruments assigned to the projects. This special privilege is defined in the user properties in CompassCDS Configuration Manager.

The user, group, and project names are defined in CompassCDS Configuration Manager.

The name, group, and project for the user are displayed in the CompassCDS status bar, at the bottom of the main screen.

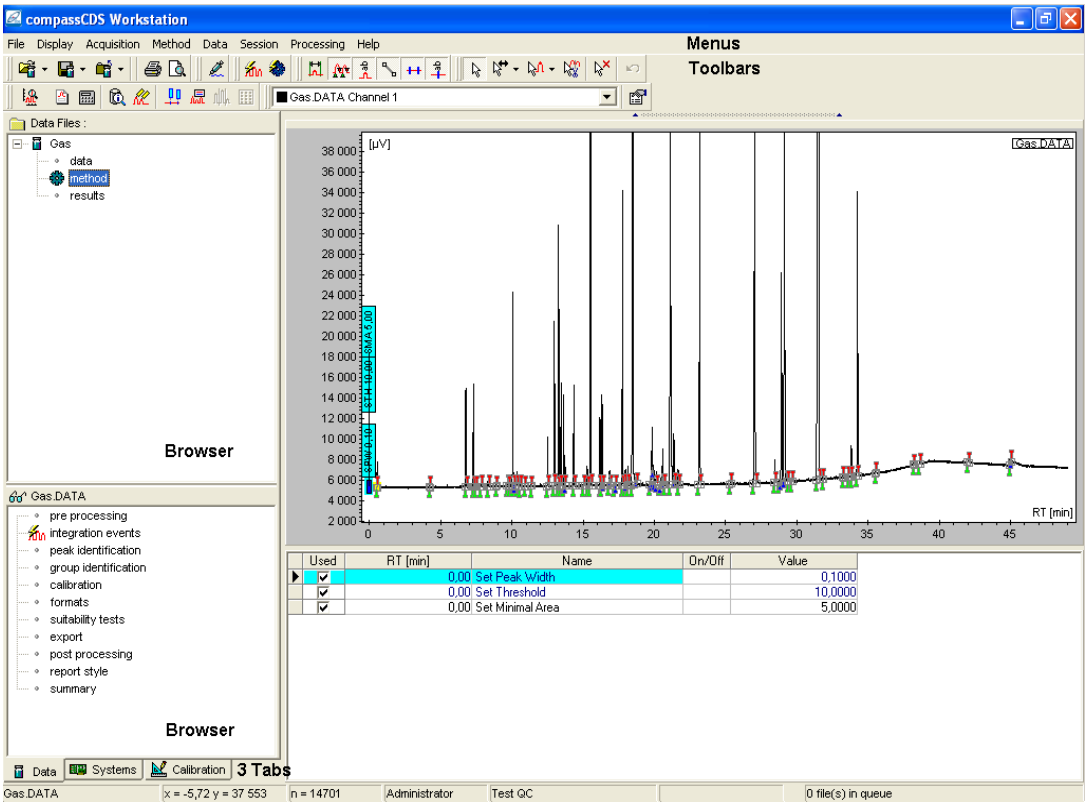
In order to change the name of the user connected or to change the group, it is necessary to logon again: Select SESSION / NEW LOGIN from the menu and a new connection window will appear as for the first logon session to CompassCDS as described above.

Any user with administrator rights can change passwords in the CompassCDS Configuration Manager. However, a user can change his password in the CompassCDS using the menu SESSION / CHANGE PASSWORD, if the user has been assigned the right to modify the password (this option is defined in the user properties in the CompassCDS Configuration Manager).

Screen Construction

The CompassCDS screen consists of a main menu, toolbars for specific tasks, a browser, three tabs, and a status bar.

The main menu provides access to most of the software functions. However, more specific tasks can be performed using the toolbars. The popup menus also provide access to many functions. Click the right mouse button within the window of interest to make the popup menu appear. All tables and graphics use popup menus.



The bar displayed above the chromatogram

May be used to hide the chromatogram, and when selected in the browser, this can be useful to display in full page the content of a selected part of the chromatogram's method. This bar is only active in post run data files.

Main Menu

Available Menus:

File menu- manages the files and configures the software and the printing.

Display menu- displays or hides toolbars; the audit trails and configures chromatogram view parameters.

Acquisition menu- starts a single acquisition, a baseline monitoring or a Remote Sequence (see page 139).

Method menu- configures the method.

Data menu- manages opened chromatograms: selection of chromatograms and viewing of chromatogram properties.

Session menu- displays information about the connected user and enables a change in logon.

Processing menu- recalculates or reprocesses the results of a chromatogram.

Help menu- provides quick access to information about software features.

The Toolbars

The toolbars provide rapid access to most CompassCDS functions. These toolbars can be displayed or hidden.

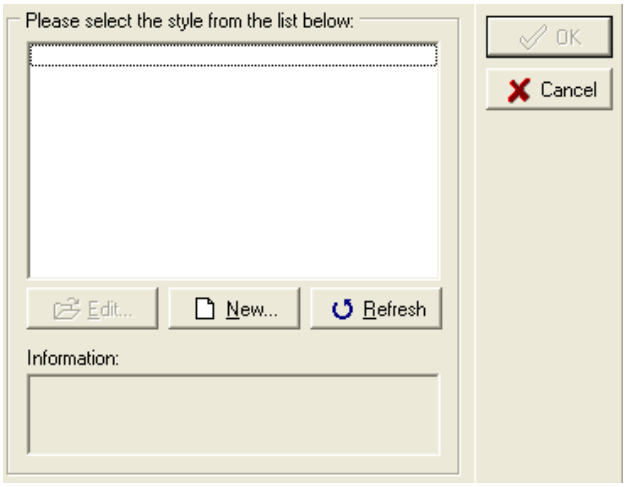
Select the menu option DISPLAY / TOOLBARS, and a window appears with a list of all toolbars that can be hidden or shown. Simply check the box next to the named toolbar in order to display it, each unchecked box indicates that the toolbar will not be displayed.

File Bar

This toolbar provides access to the file management features: open, save, close, printing, lock and Esign. These functions are available for chromatogram, method, sequence, reprocessing list.

Once a chromatogram is selected or has been opened, the first three icons can open, save, or close chromatograms. In the same way, when opening or selecting a method, a sequence a calibration curve, a reprocessing list etc. the three icons will manage the corresponding file, and their properties are modified accordingly. For example: to open a method and to open a sequence.

: To generate a PDF file on the template of the CompassCDS Report Editor report style defined in the “Report style” part of the method. The file has the name of the chromatogram plus the creation date and time with a PDF extension. If the chromatogram is signed electronically, “signed” is mentioned in the PDF file name (after the name and the date and time). To open the PDF generated file, use Acrobat reader (free on the web site www.acrobat.com) and included on the CompassCDS CD-ROM, or any PDF compatible reader utility : If a chromatogram is selected, the associated report (report style part of the method) is printed. If a method or a calibration curve is selected, the following screen is displayed:



The User selects a defined report in the list. The user can edit it by pressing the Edit button, create a new one by pressing the NEW button, or refresh the list by pressing the Refresh button.

: To have a preview of the report before its printing.

: These features are displayed only if corresponding profile is associated to the connected user. Use them to lock or unlock chromatograms files.

Electronic Signature Bar

This toolbar displayed only if the corresponding profile is associated to the connected user, provides access to (in order):

: The chromatogram signature option.

: The signature of a batch of chromatograms option.

: The list of signatures made on a chromatogram.

Display Bar

This toolbar provides access to (in order):

: to display the identification window of identified peaks centered on the experimental retention time, (if the user has defined reference peaks, and that a peak which has a theoretical retention time defined in the identification table of 3 minutes and has an actual retention time of 4.2 minutes, the window displayed is centered around 4.2 minutes). The user has to place the mouse cursor onto the name of a peak in the peak identification table to display its identification window.

: To display the start and end markers of integrated peaks.

: To display annotations of peaks (it can be the name of the peak, its retention time, etc., according to what is selected in the chromatogram annotation bar, or in the format/chromatogram section of a method).

: To display the baseline.

: To display the integration event markers.

: To display the integration event annotation selected in the chromatogram annotation bar, or in the format/chromatogram section of a method.

Chromatogram Annotation Bar

Use this toolbar to select the way to display the chromatogram on the screen.

This toolbar provides access to (in order):

: To display the Workspace, used to define the type of chromatogram view (overlay, stack, full screen), and the scale.

: To display the properties of a peak: distribution of acquired points, inflection points, etc.

: To display the audit trail of the selected object.

: To configure the way to annotate peaks.

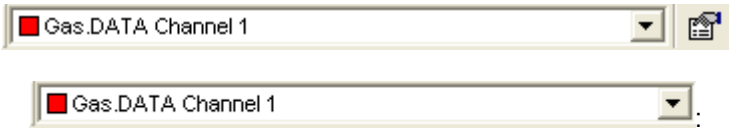
: To configure the way to annotate integration events.

: To configure annotations and markers displayed on the chromatogram.

Acquisition Bar

Starts Quick Start

Data Bar



Chromatogram name: allows the selecting and displaying of an opened chromatogram.

: Chromatogram properties: to display the properties of a chromatogram: variables, information, sample properties, etc.

Processing Bar

: To reintegrate a chromatogram after changes: In the integration part, calibration (if it is an unknown only), peak and group identification.

: To reprocess a chromatogram, this function allows you to perform all the functions, accessible from the method.

Manual Integration Bar

(refer to page 170)

This toolbar provides access to (in order):

	To select the peak for which the integration has to be modified.
	To move the peak markers.
	To add a new peak by defining its start and end.
	To split a peak into two peaks.
	To remove a peak
	To merge two peaks
	To delete the last manual operation performed.

Every manual change executed is listed in the part results/manual operations of the chromatogram.

NOTE: To unlock a toolbar and make it a separate moveable window, click at the left side of a toolbar then drag it to the desired location.

The Browser

The browser is displayed at the left part of the application window to permit viewing of opened files names.

The browser can be hidden. If it is not visible, select the menu option DISPLAY and check BROWSER.

At the bottom of the browser are three tabs: Data, Systems, and Calibration. Click on Data to view the chromatograms, sequences, methods and the reprocessing list that are opened. Click on Systems to display the running acquisitions. Click on Calibration to edit the calibration curves.

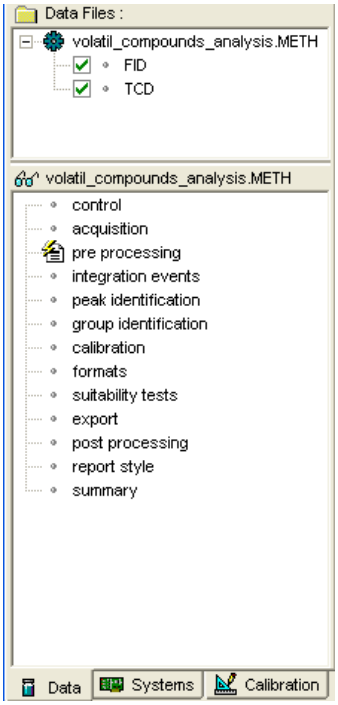
Press the right mouse button on any item displayed in the browser to view a popup menu to provide faster access to options when performing certain tasks.

To Display a Method

Select the menu option FILE / OPEN / OPEN METHOD and double-click on the file name to be opened.

The name of the method is displayed in the browser. The method can be a multi-channel method. In this case, the sub-methods for each channel are shown above the name of the method. By clicking on one or another channel, the right panel display will be updated corresponding to the selected channel.

The method is composed of several sections (Control, Acquisition, Integration, etc.). Each section can be displayed in the right panel by clicking in the bottom part of the browser.



The name of the method, under which the channel sub-methods are listed, is also displayed in the space between the two parts of the browser.

Click the right mouse button on the method to view its popup menu. The popup menu of a method is:

CLOSE METHOD	To close the method
SAVE METHOD	To save the method
SAVE METHOD AS	To save a method under a new name.
SAVE METHOD AS TEMPLATE	To save the method as a template.
PRINT	To print the method report.
AUDIT TRAIL	To display the audit trail of the method.

The popup menu of the grids (displayed in the right part of the screen) contains a Copy option that allows the grid content to be copied for pasting into another application (Word, Excel).

To view a Chromatogram

Select the menu option FILE / OPEN / OPEN CHROMATOGRAM and double-click on the file name to open.

The name of the chromatogram is displayed in the browser. A chromatogram is saved with the method used to process it and the results.

- Click on Data to view the chromatogram in the right panel.
- Click on Method to display the method. The method is composed of several sections (Control, Acquisition, Integration, etc.). These sub-methods are displayed in the right panel by clicking on them in the bottom part of the browser.

NOTE: To hide the chromatogram when displayed above the method, uncheck the menu option DISPLAY / DATA VISIBLE, or click on the bar above it:

- Click on Results to view the calculation results in the right panel. The results include the manual operations, peak table, and group table. Click on each element to obtain the corresponding results on the right panel

Press the right mouse button on the chromatogram name displayed in the browser to view its popup menu. The following options are available.

CLOSE CHROMATOGRAM	To close the chromatogram without using the Close chromatogram window.
SAVE CHROMATOGRAM	To save the chromatogram.
SAVE METHOD AS TEMPLATE	To save the method of the chromatogram as template.
PRINT	To print the chromatogram report.
DATA VISIBLE	Check or uncheck this menu to show or hide the chromatogram in the right panel, when method or results parts are selected.
AUDIT TRAIL	To view the processing history of the chromatogram, a list of the operations made with the chromatogram is given.
CHROMATOGRAM PROPERTIES	View the chromatogram properties ( ), and parameters such as the sample mass, the internal standard mass and all the global variables, including the user input variables.

Press the right mouse button on the data part of the chromatogram in the browser, the DATA VISIBLE option is available in the popup menu.

Press the right mouse button on the method name of the chromatogram in the browser to view its popup menu. The following options are available.

UPDATE METHOD	To update the last method used to reprocess the chromatogram with the chromatogram processing parameters
SAVE METHOD AS	To save the method as a new method, with a new name.
SAVE METHOD AS TEMPLATE	To save the method of the chromatogram as template
AUDIT TRAIL	To view the processing history of the chromatogram. A list of the operations made with the chromatogram is given.

To view a Sequence

Select the menu option FILE / OPEN / OPEN SEQUENCE and double-click on the file name to open.

The name of the sequence is displayed in the browser. Click on it to display the sequence in the right part of the application.

Press the right mouse button on the sequence displayed in the browser to view its popup menu. The popup menu of a sequence is:

CLOSE SEQUENCE	To close the sequence: it is not possible to close a running sequence.
SAVE SEQUENCE	To save the sequence.
SAVE SEQUENCE AS	To save the sequence under a new name, so that the original sequence file is not lost (overwritten).
PRINT	To print the sequence.

To view a Reprocessing List

Select the menu option FILE / OPEN / OPEN REPROCESSING LIST and double-click on the file name to open it.

The name of the reprocessing list is displayed in the browser. Click on it to display the reprocessing list in the right part of the application.

Click the right mouse button on a reprocessing list displayed in the browser to view its popup menu. The popup menu of a reprocessing list is:

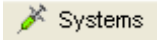
CLOSE REPROCESSING LIST	To close the reprocessing list.
SAVE REPROCESSING LIST	To save the reprocessing list.
SAVE REPROCESSING LIST AS	To save the reprocessing list under a new name, so that the original reprocessing list is not lost (overwritten).
PRINT	To print the reprocessing list.

To View an Acquisition

Click on the System tab set at the bottom of the browser. The list of all accessible chromatographs (dependent upon user access rights and group/project definition) is displayed in the browser.

For each chromatograph (or system), the active chromatogram, as well as system status (particularly interesting if the system has a fully controlled autosampler) and general information about the run can be viewed during the live acquisition.

This information can be displayed “by system” or “by type”:

Press the 

button to view all information concerning one system in the same window. When this button is pressed, choose which information will be displayed for each system by checking the corresponding objects.

Press the By type button to view only one type of information (acquisition or status), for a few or all of these systems (check the corresponding systems).

A maximum of 2 chromatograms or 2 status displays can be viewed by page.

Click on the right mouse button on an item displayed in the browser to view its popup menu.

To view a Calibration Curve

Click on the Calibration tab at the bottom of the browser.

Select the menu option FILE / OPEN / OPEN CALIBRATION CURVE and double-click on the file name in order to open the selected file.

A calibration curve consists of several curves, one for each compound calibrated in the chromatogram. In the browser, click on the compound to display the corresponding curve in the right panel

All previous versions of a calibration curve are not completely deleted, but archives can be created if the user allows it, (defined in CompassCDS Configuration Manager). The archives can be sorted by date or by name:

- Press the Arch / button to sort them by compound.
- Press the Arch / button to sort them by date.
- Press the Cur. button to view the current curves.

NOTE: The archiving date of a file corresponds to the date at which the calibration curve has been replaced, i.e., the creation date of the new curve. The calibration curve creation date appears in the right screen.

The Status Bar

The status bar at the bottom of the main screen displays information about the software status:

File name zone: Displays the name of the selected file (and channel in the case of multi-channel chromatograms and methods).

Process zone: Displays a progress bar during a calculation or any other task indicating that the system is busy. When the system is available, by pointing the cursor inside a curve, the coordinates of the cursor position are also displayed in this zone.

Point's number (n=): If a chromatogram is selected, this field indicates the number of points constituting this chromatogram, or if only a part of the chromatogram is displayed (zoom), the number of points contained in this part of the signal.

User name zone: Displays the name of the current user.

Group-project zone: Displays the group and the project names of the current session. In the case of an "all projects" connection, only the name of the group is displayed.

Method Name: If a chromatogram is opened, an additional field mentioning the name of the last method used to process the chromatogram is added after the Group/project.

Waiting process: Indicates the number of processes that have to be performed, or the last process done.

These different fields can be empty, according to the tab selected (Data, Systems, Calibration), the process running or the selected object.

The Shortcuts

Many shortcuts have been defined within CompassCDS, which will be helpful in order to work quickly using the keyboard.

Note that these shortcuts are also displayed within CompassCDS menus.

Warning: The numbers used in the shortcuts cannot be entered from the numeric keypad on the keyboard.

Displaying

The following shortcuts keys of the software are listed below:

F1	Press this key to display the online help menu.
F2	Press this key to display the chromatogram properties in which the sample mass the internal standard quantity and all the global variables (including user input variables) are displayed and can be modified.
F3	Press this key to display the workspace in order to change the full scale or zoom within the chromatogram.
Ctrl+F3	Press these keys to display the peak properties displaying some peak variables.
F9	Press this key to display the Data of the browser window (the panel where the acquired chromatograms, the methods and the sequences are displayed).
F10	Press this key to display the System of the browser window that contains the actively running acquisitions. If this button is pressed in the System panel, the buttons Systems and By type will be selected one after the other.
F11	Press this key to display the Calibration of the browser window, when the calibration curve is displayed. If this button is pressed when a calibration curve is displayed, the buttons Cur, Arch/compound and Arch/date will be selected one after the other.

Run

The following shortcuts quickly perform certain actions:

F5	Press this key to start the integration and the identification of the selected chromatogram.
F6	Press this key to open the Reprocessing window.
F8	Press this key to open the Quick Start window.
Ctrl+Alt+4	Use these keys to start a sequence.
Ctrl+Alt+5	Use these keys to start a reprocessing list.

File

The following shortcuts provide rapid access to certain actions available in the file menu:

Alt+F4	Press these keys to quit CompassCDS Chromatography Data System.
Ctrl+F4	Press these keys to close the selected chromatogram
Shift+Ctrl+F4	Press these keys to close all the files opened in CompassCDS Chromatography Data System
Ctrl+S	Press these keys to save all the files opened in CompassCDS Chromatography Data System
Ctrl+P	Press these keys to print a report for the selected chromatogram with the report style selected in the method.
Alt+Ctrl+F4	Press these keys to display a preview of the report for the selected chromatogram
Ctrl+H	Press these keys to view the chromatogram.
Ctrl+W	Press these keys to access the report style open file box.

To open, close, save, or create a new file, use the following shortcuts:

Ctrl+1	Press these keys to access the chromatogram open file box.
Ctrl+2	Press these keys to access the method open file box.
Ctrl+3	Press these keys to access the calibration curve open file box.
Ctrl+4	Press these keys to access the sequence open file box.
Ctrl+5	Press these keys to access the reprocessing list open file box.
Ctrl+6	Press these keys to access the summary report open file box.
Ctrl+7	Press these keys to access the spectral library edition window (available if you have a Diode Array Detector).

To create a new file, use the Ctrl+Alt keys plus the number defined above. Note that it is not possible to create a new chromatogram or a new calibration curve.

To save files, use the Shift+Ctrl keys plus the number defined above.

To save a file under a new name, use the Shift+Ctrl+Alt keys plus the number defined above. Note that it is not possible to save a chromatogram or a calibration curve under a new name.

To close files, use the Shift+Alt keys plus the number defined above.

Result

The following shortcuts will display the results of the selected chromatogram:

Ctrl+M	Press these keys to display the manual operation history.
Ctrl+A	Press these keys to display the peak result table.
Ctrl+U	Press these keys to display the group result table.

Annotation

The following shortcuts will modify the chromatogram displays:

Ctrl+Alt+C	Press these keys to open the chromatogram annotation screen in order to modify all the chromatogram annotations (Including the following ones).
Ctrl+Alt+E	Press these keys to modify the integration events display within the chromatogram.
Ctrl+Alt+K	Press these keys to modify the peak annotations display.
Ctrl+Alt+I	Press these keys to display or hide the peak identification windows.
Ctrl+Alt+M	Press these keys to display or hide the peak markers.
Ctrl+Alt+N	Press these keys to display or hide the peak annotations.
Ctrl+Alt+B	Press these keys to display or hide the baseline.
Ctrl+Alt+V	Press these keys to display or hide the integration event markers.
Ctrl+Alt+T	Press these keys to display or hide the integration events.

Method

The following shortcuts are used to display different parts of the method.

F7	Press this key to display the Variable editor.
Ctrl+L	Press these keys to display the control method section.
Ctrl+Q	Press these keys to display the acquisition method section.
Ctrl+N	Press these keys to display the pre-processing method section.
Ctrl+I	Press these keys to display the integration method section.
Ctrl+K	Press these keys to display the peak identification method section.
Ctrl+G	Press these keys to display the group identification method section.
Ctrl+B	Press these keys to display the calibration method section.
Ctrl+T	Press these keys to display the suitability tests.
Ctrl+F	Press these keys to modify the peak report, group report and chromatogram formats.
Ctrl+E	Press these keys to display the export method section.
Ctrl+F	Press these keys to modify the peak report, group report and chromatogram formats
Ctrl+O	Press these keys to display the post-processing method section.
Ctrl+R	Press these keys to display the printing method.
Ctrl+Y	Press these keys to display the summaries method.

Sequence and Reprocessing List

Ctrl+↵ (enter) Press these keys to display the information available with the ··· button.

File Structures

There are several different file types used in CompassCDS (chromatogram, method, sequence, etc.). Most files can be opened and displayed using the browser.

Chromatograms

A chromatogram consists of:

Raw data: The acquisition data points.

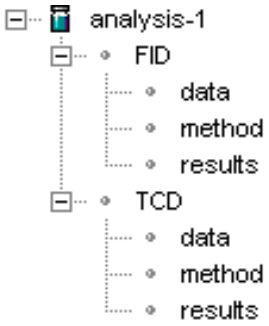
Method: Indicates which is the last method used to process the chromatogram. Control and acquisition methods are never modified during a reprocessing; they are defined at the time of acquisition.

Results: The results group, peak tables and the manual modifications list, if any.

Audit Trail: Traces the history of all methods, which have been used to process the chromatogram and the associated results.

After the chromatogram acquisition, the user can modify its method (integration parameter, identification…) and recalculate the results using these new parameters. The previous method will be kept in the archive, and the new, updated method will be saved. It is also possible to reprocess a chromatogram with a totally different method (Menu option PROCESSING / REPROCESS).

One data file (XXX.DATA) is created by injector, which means that if the chromatographic system is defined with two injectors, two data files are generated by analysis. If several channels are defined by injector, the chromatogram data files generated are composed of several signals. The following picture represents the display of the chromatogram in the browser, in the case of a system with two channels.



Methods

A method consists of several sections:

Control method: Contains the parameters used to execute the acquisition: acquisition rate, start mode and, in the case of a fully-controlled system, the configuration parameters and programs of the chromatograph modules.

Acquisition method: The default parameters will be automatically displayed in the acquisition screens (Quick Start and sequence): run time, run name, etc. It is possible to modify these parameters for every acquisition using these screens.

Preprocessing method: This section contains the blank chromatogram, if any.

Integration method: List of the automatic integration events and the parameter set times

Identification method: The identification parameters of the peaks and groups.

Calibration method: This option is used to set the quantification parameters (Response percentages, external standard etc.) and also to set the calibration curve parameters, if any.

Formats: This feature enables definition of a format for group reports, peak reports, and chromatograms. Formats can also be defined in the properties: right click in the chromatogram, peak or group report and then select the PROPERTIES option.

Export method: The nature, name, path, and content of the method file, which will be exported during the reprocessing is defined.

Suitability tests: This section allows the setup of suitability tests on the defined variables. If one of the tests fails, CompassCDS will display on the screen and/or print in the report, the warning message as defined by the user.

Post processing: Used to run programs or macros after the completed processing of the chromatogram. Be careful to close the files containing the macros before launching them or processing will not be possible.

Print method: Displays the name of the report style.

Summary: Displays the summary or the summary name(s) selected.

File Management

There are two ways to manage the files: using the FILE menu or the File toolbar:

File Menu

Creation of a New File

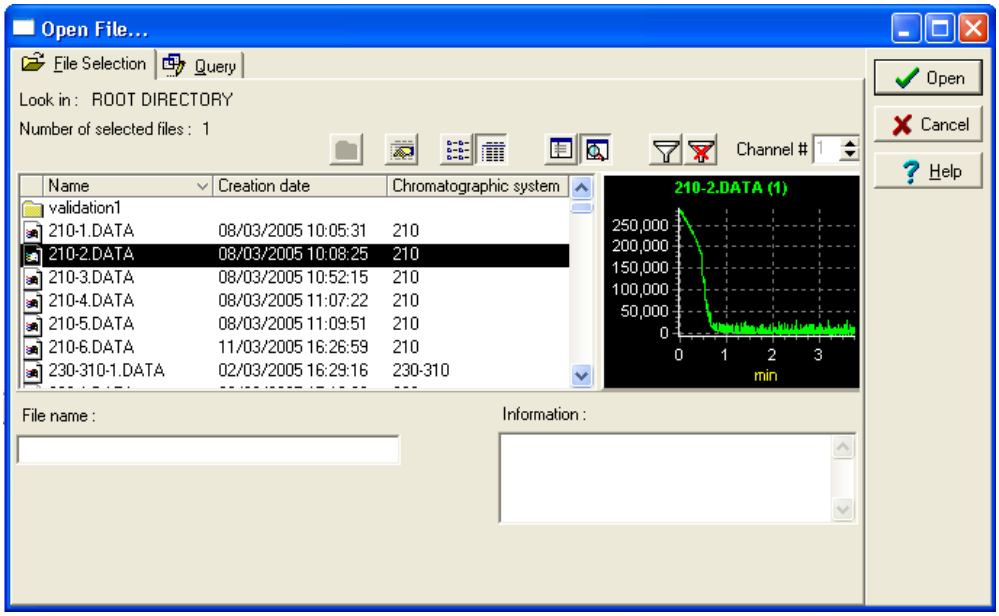
Use the pull-down menu option FILE and then select NEW / NEW METHOD, NEW METHOD FROM TEMPLATE, NEW REPORT STYLE, NEW SEQUENCE, NEW REPROCESSING LIST, or NEW SUMMARY REPORT, to create the corresponding new file in CompassCDS.

For each type, wizards will guide the user through creating the new file.

Open a File

The menu options FILE / OPEN will open the chromatograms, method, report style, calibration curve, sequences, reprocessing lists, summary report.

Each file uses its own “open file” dialog boxes, all based on the same template.



The Open file dialog displays the list of those files visible in the directory associated with the group (when the user is logged on to “All projects") or with the project (when the user is logged on to a specific project).

It is possible to access the sub-directories: double-click on the folder icon ( ). While in the sub-directories, the path is displayed at the top of the window (‘look in :’). It is possible to return to the previous directory by using the root directory button .

NOTE: The Chromatogram open file box allows the user to open chromatograms generated by different software’s: CompassCDS (.DATA) and also AIA (.CDF) files.

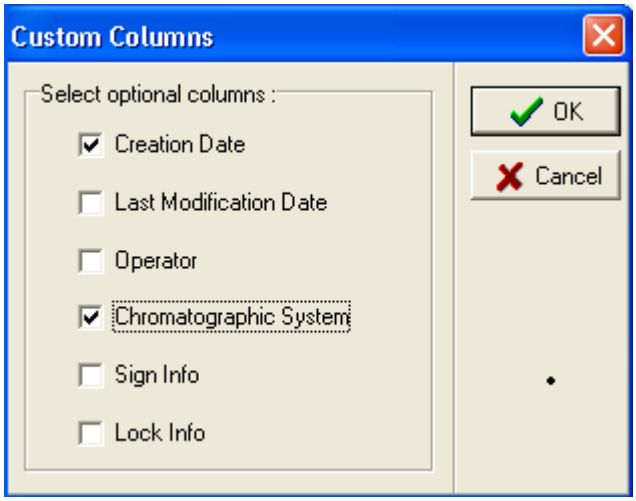
Open file toolbar:

	Use this button to return to the root directory.
	Use this button to customize the columns to be displayed.
	Use this button to display only the list of the files.
	Use this button to display the files with details (acquisition date), etc.
	Use this button to display only files.
	Use this button to display files and a preview of the selected file (only for chromatograms).
	Use this button to apply the filter defined in the Query page
	Use this button to deactivate the filter.

Sorting files

It is possible to sort files by name or creation date in either increasing or decreasing order by clicking in the column header. A down arrow indicates that the files are sorted in increasing order, while an up arrow shows that the files are sorted by decreasing order.

It is also possible to display and to sort files according to other criteria: click on the custom column button , the following window is displayed



User puts a checkmark into the columns to display: creation date, last modification date, operator, chromatographic system, sign info, or lock info associated with the files. The sign info and lock info are available only for chromatograms and inform user that the file has been signed off and locked.

The Open file box size is adjustable, to allow the viewing of all the columns.

NOTE: The creation and modification date correspond to Windows date. For example, if you overwrite a file (when you have the right to overwrite existing files) the creation date is not updated and will correspond to the date of the first creation with the same name.

Selecting file:

To scroll through the file list, use the keyboard arrows or the cursor on the vertical scroll bar.

The selected file is displayed in "BLUE" and, at the same time, a compressed image (if possible) of the file and file information appears at the right of the window. The content of this information is entered during file creation (New method, New sequence). For chromatograms, the information has to be entered in the "Quick Start" window or in the sequence. This field is also accessible when processing a "Save as" file.

To select or deselect several files at the same time, use the SHIFT or Ctrl keys combined with left mouse clicks, as in Windows Explorer. When all the files to be opened are selected, press the OK button.

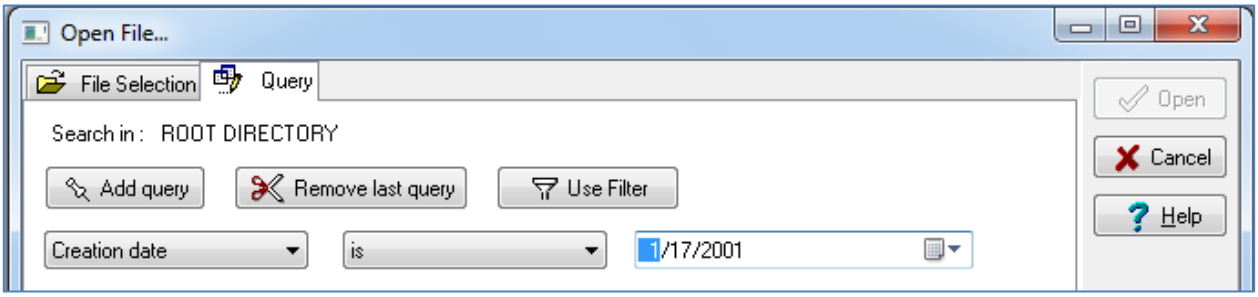
NOTE: It is not possible to open several methods, summary reports or calibration curves at the same time.

Chromatogram preview

If a preview of the chromatogram is displayed in the Open file window, it is possible to zoom in on this image, and magnify it using a click and drag with the left mouse button from the top left-hand corner to the bottom right-hand corner of the area. It is also possible to scroll the zoomed area by holding down and then moving the right mouse button. To zoom out, click and drag the left mouse button from the bottom right-hand corner to the top left-hand corner.

Queries

The Query page allows user to define filters. Once a filter is activated, only the files which correspond to the query's specific criteria are displayed in the File selection page.



Several queries can be made simultaneously. To add a query, click on the Add Query button. To remove the last query, click onto the remove last query button. To apply queries, click onto the Use filter… button. Queries are connected by the 'AND' logical operator, that means all the defined queries must be satisfied to select a file.

Files can be sorted according to:

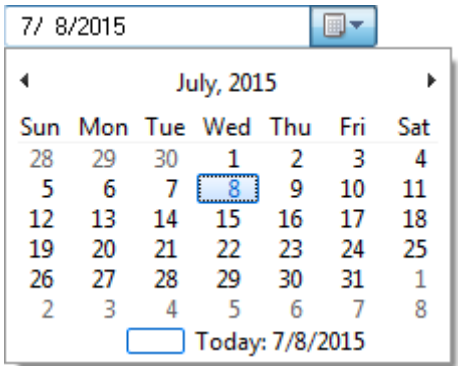
- Acquisition date
- Last modification date
- Operator name
- Information content
- Chromatographic system name associated to the file
- Sign info
- Lock info

The options for the second and third fields depend on the query being specified.

Sort according to dates:

The second field options are:

- is
- is before
- is after
- the date choice is made by activating the third field:



Sort according to: operator name, information field, chromatographic system name:

The second field options are:

- is (this option is not available for information field)
- contains
- begins with
- ends with

The user enters the desired text in the third field.

Sort according to sign info and lock info:

The second field is set to 'is'.

The third field options are: signed file / unsigned file and locked file / unlocked file.

To view the result of the queries, click on the Use Filter… button, the 'File selection' tab is then displayed, listing the files which satisfy the queries. To cancel queries, click on the deactivation icon filter . To again apply the queries defined in the 'Query' tab, click on the use filter icon .

Note that to sort files faster, the user can enter in the 'File name' field of the main screen: The first letters of the file name to open: only files whose name begins by those letters are displayed.

- *letters: only files whose name ends by these letters are displayed.
- *letters*: only files whose name contains these letters are displayed
- *.XXX: only files whose extension is XXX are displayed (only for chromatogram file, allowing the opening of .DATA, .CDF files)

Save a file

Two possibilities exist: save a file with same name (overwriting the previous one) by using the menu FILE / SAVE / SAVE file type, or save the file with another name by using the menu

FILE / SAVE AS / SAVE / file type AS. In both cases, the CompassCDS Chromatography Data System prompts to save the file type corresponding to the active file.

When several files of the same type are opened, the currently selected file will be saved. Therefore, click first on the file to be saved in the browser, then select FILE / SAVE / SAVE file type.

Each file uses its own 'SAVE AS file' box, based on the same template. The Save file window displays a list of the files already created in the directory associated with the group (when the user is logged on to "All projects") or with the project (when the user is logged on to a specific project).

It is possible to access the sub-directories by double-clicking on the corresponding icon ( ). Once in the sub-directory, the path is displayed at the top of the window ('Look in :') and it is possible to return to the previous directory using the Root directory button .

Enter the name of the file in the File Name part. Enter the corresponding information in the corresponding zone and then press the Save button.

Selecting an existing file name will overwrite the existing file. An on-screen warning message will appear since the file that is about to be overwritten will be lost and unrecoverable.

For Chromatogram file, two saving functions are available: 'save method as', allowing to save the chromatogram method as a separate file (.METH) with another name than the one of the method

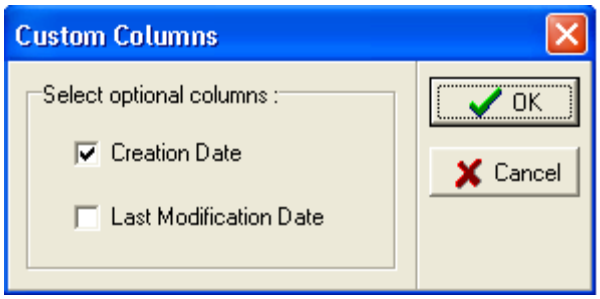
associated to the chromatogram; ‘save method’ allowing to overwrite the method associated to the chromatogram.

File/Save Toolbar

	Use this button to return to the root directory.
	Use this button to customize the columns to be displayed
	Use this button to display only the list of the files.
	Use this button to display the files with details (acquisition date).

It is possible to sort files by name or creation date in either increasing or decreasing order by clicking in the column header. A down arrow indicates that the files are sorted in increasing order, while an up arrow shows that the files are sorted by decreasing order.

It is also possible to display and to sort files according to other criteria: click on the custom column button , the following window is displayed:



The user puts a checkmark into the columns to display: creation date or last modification date.

NOTE: The creation and modification date correspond to Windows date. For example, if you overwrite a file (when you have the right to overwrite existing files) the creation date is not updated and will correspond to the first file creation.

The menu options FILE / SAVE ALL will save all the files that are opened in CompassCDS.

Close a File

The FILE **/** CLOSE / CLOSE Type of file to close menu is active only if a file of this type is currently opened in CompassCDS.

When several files of the same type are opened, the currently selected file will be closed. Therefore in the browser, first click on the file to be closed, then select FILE / CLOSE / CLOSE type of file.

The option to close several chromatograms at the same time is available. Therefore, when choosing the menu option CLOSE CHROMATOGRAM, a window is displayed, which lists the names of all open chromatograms. Select each of the chromatograms to be closed, then press OK. All of the selected chromatograms will be closed at the same time. It is also possible to select or deselect all of the chromatograms using the Select all button.

The menu option FILE / CLOSE ALL will close all of the files that are currently opened in CompassCDS.

Competitive File Access

If a user tries to open a file which is already opened in CompassCDS by another person, a message advises the user that the file can only be opened in read-only mode. No modification can thus be saved, therefore the Save button of a read-only file is inactive.

Chromatogram: A read-only chromatogram can be modified either by the "Integrate" (F5) function or by manual integration or identification, but it cannot be saved. CompassCDS allows the printing of the modified results. A report corresponding to an unsaved data file is printed with a "Data Not Saved" background.

Method: A read-only method can be modified but not saved.

Sequence: When a sequence is in read-only mode, only column customization and sequence printing are allowed. Other modifications are not allowed (add/delete lines, clear sequence, start sequence…)

Reprocessing list: When a reprocessing list is in read-only mode, only column customization and reprocessing list printing are allowed. Other modifications are not allowed (add/delete lines, clear reprocessing list, start reprocessing list…)

Summary report: When a summary report is in read-only mode, it can be printed, but the chromatogram number and variables cannot be modified.

Report style: A read-only report style can be modified, but not saved.

Calibration curve: A message advises the user when the curve is already use by another user.

Generally speaking, when a file is already opened, CompassCDS forbids the creation of a new file with the same name.

The "Save as" function also forbids to keep the same name. But, chromatogram method can be saved with the same name if the "Save chromatogram method" CompassCDS Configuration Manager profile has been selected. Select the "Save chromatogram method" from the popup menu of the chromatogram method in order to save the chromatogram method under the same name.

File Toolbar

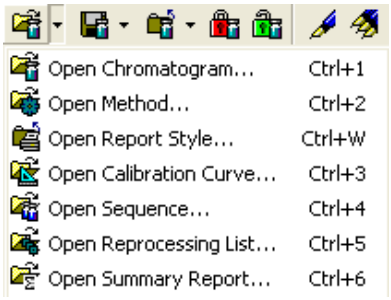
The icons also provide chromatogram management as in the corresponding menus. The only difference is that the icons provide faster access.

The first icon will open files, the second will save current files, and the third will close files.

The graphic appearance of the toolbar (three first buttons) changes slightly according to the active file type currently loaded in CompassCDS. For example, if chromatograms are being managed, the open file icon will appear as . If methods are being managed, the icon will appear as . When working with sequences, the icon will appear as with calibration curves, the icon will appear as .

When working with the reprocessing list, the icon will appear as .

If the current icons are displayed for chromatogram management, it is possible to change this display. For example, to open a calibration curve, click on the arrow at the icon's right, then select the correct sub-menu:



The appearance of the toolbar is changed when a file is opened, saved, closed, or when a file is selected.

File Storage and File Extensions Generated by CompassCDS

Files are stored in directories whose paths are defined in CompassCDS Configuration Manager.

Each file type generated by CompassCDS uses its own extension, thus making it easy to find using the Windows Explorer.

- Chromatogram: .DATA
- Method: .METH
- Sequence: .SEQU
- Reprocessing list: .REPL
- Report style: .STYL
- Method report style: .STYM
- Calibration report style: .STYC
- Calibration curve: .CALB
- Summary report: .SUMR

The following characters are not allowed in a file name \ / : * ? " < >.|

The chromatograms, methods, sequences and reprocessing lists files are stored in the project root directory. Calibration curve, summary report and report style files are stored in the group root directory, thus allowing their use in several projects belonging to the group.

If a method is defined in a project, and that user wants to use it in another, the user must save it "as a template method" and once logged in the right project, the user must create a "new method from template" (see page109). It is recommended that the user refrain from copying a method from a directory to another. Indeed since, a method is linked to a project at its creation. All chromatograms acquired with this method are stored in the project directory. Copying this method in another project directory, via the Windows Explorer, will introduce confusion; all newly acquired chromatograms will be stored in the original project directory and not in the new one. Nevertheless, calibration curves and report styles can be copied from one group to another and chromatograms from one project to another as well.

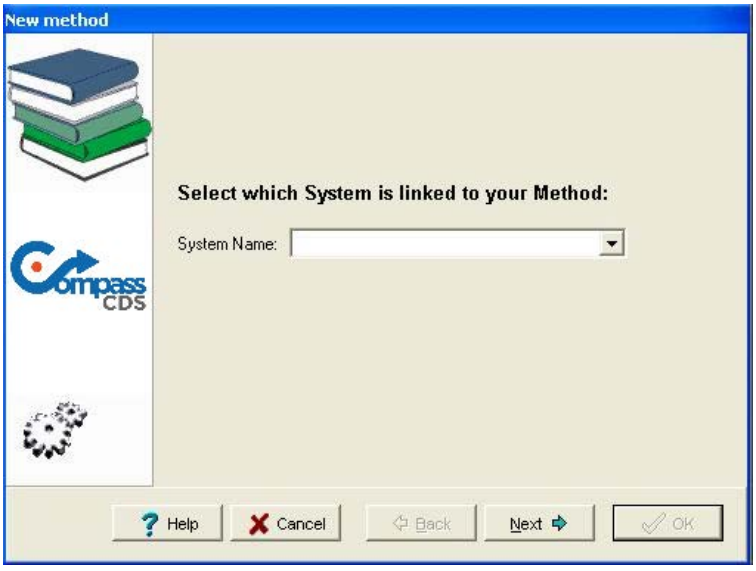
The Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and the format of results.

It is not compulsory to define all of the method sections when initially setting up an acquisition, but it is mandatory to complete the instrument control section prior to start an acquisition (especially for an automatic operation).

Create a Method

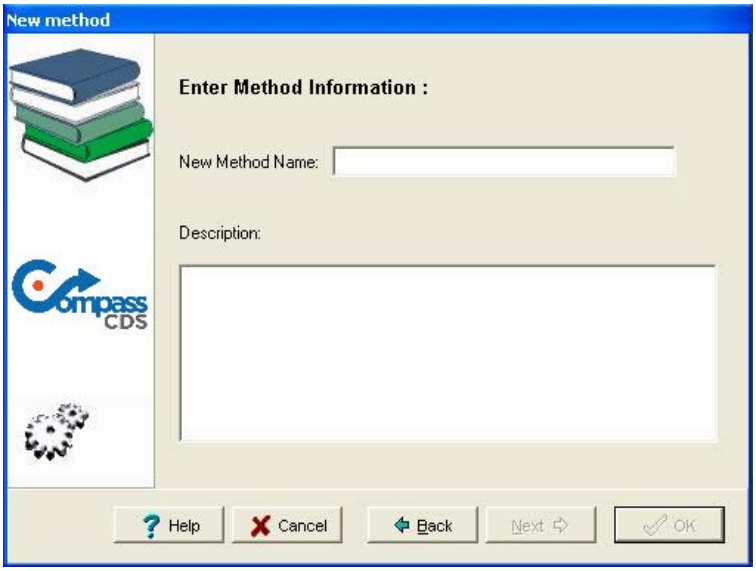
Select the FILE / NEW / NEW METHOD options from the main menu. A wizard provides assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. Thus, when starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those associated with this system.

NOTE: If the user is connected under 'all projects', the 'New method' wizard will contain one additional field to allow selection of the project.

Once these two fields are completed, the NEXT button is activated. Click on the NEXT button to move to the second step of the method creation:



Enter the new method name in the first edit box. In the description box, enter information concerning the method (optional). This will be displayed in the open file window, when the file is selected.

Once the entry of these two fields is completed, the OK button is activated. Click on the OK button, and the new method is created and will be opened with default parameters in CompassCDS.

The next step is to define each of the method sections. The instrument control section must be defined in order to start an acquisition. This is the minimum requirement. However, the other sections may be defined later, after the acquisition of a chromatogram in order to view the peak retention times.

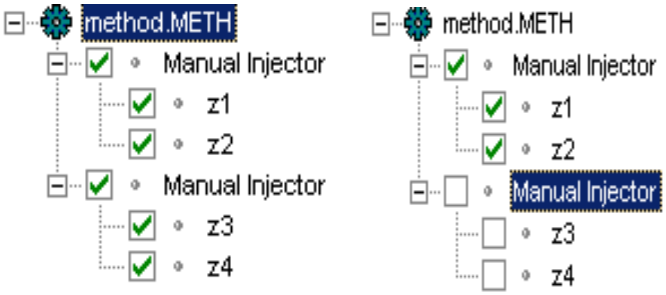
For multi injector system:

Control section is defined for the whole system. Only one control method must be defined.

Acquisition section is specific for each injector.

Other sections of the method (Pre-processing, Integration, Identification…) are specific to each detector. Parameters must be set for each detector channel.

It is possible to disconnect an injector, or channels, by unchecking them in the browser.



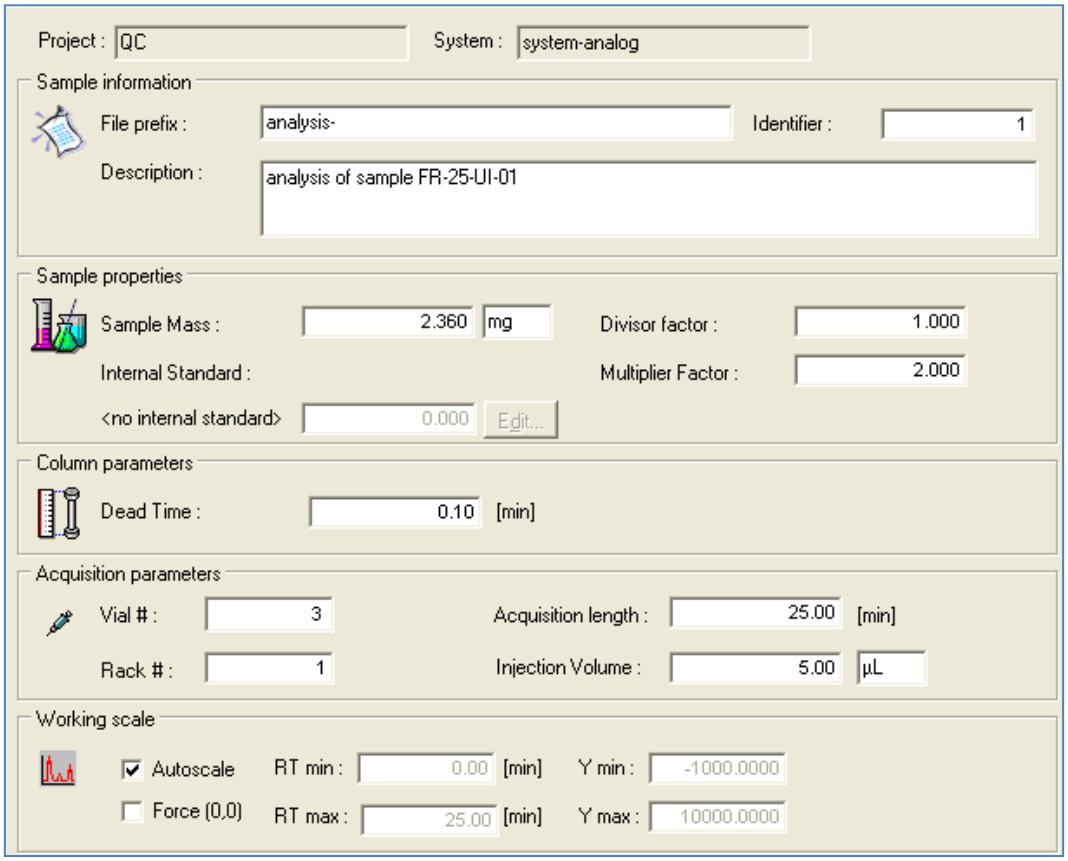
The Different Parts of the Method

Control

This section of the method depends on the chromatographic system. For fully controlled instruments (e.g., where a specific instrument control driver is used), the control section consists in all the parameters that can be set for this chromatography system.

Acquisition

In the acquisition method, default parameters are set as they will be displayed in the acquisition windows: Quick Start or sequence. It is also possible to modify these parameters before starting the acquisition.



File prefix: Specify the first part of the chromatogram name in this zone. The chromatogram name will have the identifier appended to it.

Identifier: Specify a numeric value for the second part of the chromatogram name in this zone. For example, if the file prefix is ‘Run’ and the identifier is 55, the name of the chromatogram will be Run_55.data. The identifier is incremented automatically after each acquisition in the case of single acquisitions (started using the Quick Start).

Description: Information about the run may be entered in this area. This information will be saved with the chromatogram and displayed in the open file window and in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES). The description can be a maximum number of 255 characters.

Sample mass: Enter the total mass of the sample in this field. This value can be used for the calculation of compound amounts. The sample mass variable can be used along with all the other variables available in the variable editor. Enter the mass unit in the adjacent edit box.

Internal standard: It is possible here to define default internal standard quantity (or quantities). User must previously have defined the name of the internal standard(s) in the Peak Identification part of the method and have indicated which (whose) peak(s) are internal standard(s) in the calibration part of the method. Enter then the corresponding value in the internal standard zone, or if there are several internal standards, press the Edit button.

NOTE: If the internal standard quantity changes from a sample to another, it is not advisable to enter a value at this step. The internal standard can be entered in the Quick Start window, in the corresponding column, in the sequence for an acquisition, in the chromatogram properties for single run reprocessing, or in the corresponding column in a reprocessing list.

Multiplier factor: This variable is used to multiply all the quantities calculated by the same factor.

Divisor factor: This variable is used to divide all the quantities by the same factor.

Specific Channel Parameters: This option is displayed only in the case of a multi-channel system. It allows the user to enter different Multiplier factors, Divisor factors, sample masses and working scales by channel.

Dead time: This time corresponds to the time required for the sample solvent (or any non-retained compound) to reach the detector. This time is used for the calculation of the selectivity and capacity factor.

Vial: The vial number can be entered for information only or can be used to specify which autosampler vial number should be injected.

Rack: The rack number can be entered for information only or can be used to specify the rack number that contains the vial that should be injected in the case of a fully controlled autosampler.

Acquisition length: Specify the total acquisition time in this field.

Injection volume: The injection volume can be entered for information only or can be used to specify an injection volume for the autosampler if fully controlled by CompassCDS. Enter the volume unit in the adjacent edit box.

Working scale: By default, the Y scale of the chromatogram is defined according to the maximal signal. However, in the case of a chromatogram containing a very large solvent peak, it can be useful to display only the small peaks. By un-checking the Automatic Box, it is possible to select limits to display the chromatogram during the acquisition, both on the main screen and in the report (if special limits are not set in the report). The Force (0,0) option forces the scale of the acquisition screen to display the origin (0,0), for example, to show the (offset) of a chromatogram. This function cannot be used to force the signal to go through the origin.

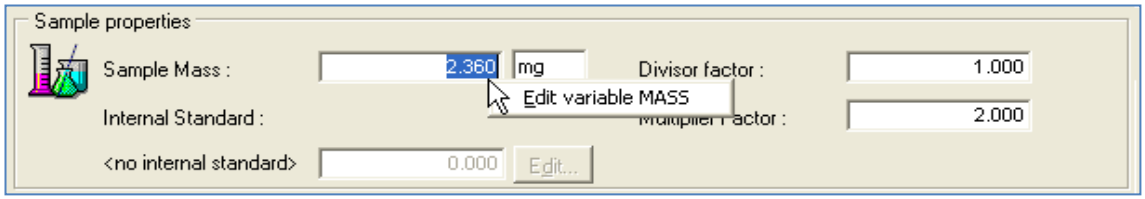
User can easily modify the format of the following displayed variables:

In **Sample Properties:** every variable

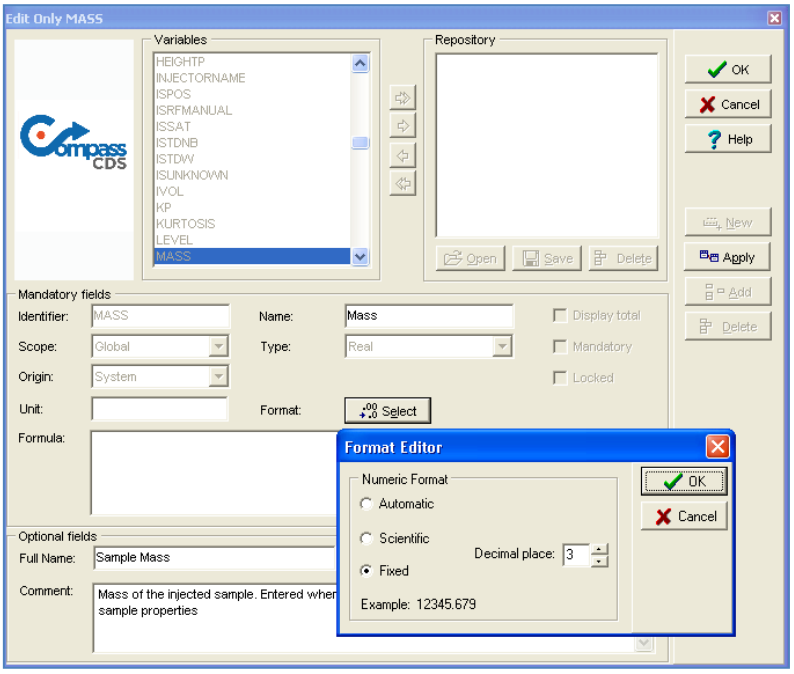
In **Acquisition parameters:** acquisition length

In **Working scale:** RT min and RT max

To change the format, put the cursor of the mouse on the box corresponding to the variable which format has to be modified, click on the right mouse button and select the option ‘Edit Variable XXX’ in the popup menu, where XXX represents the variable name.



The variable screen is then displayed, allowing only the modification of the selected variable format. For example for the sample mass, the following screen is displayed:



Note that the ‘Quick Start’ screen is almost the same as the one of the acquisition section of the method. The format of some variables displayed in the ‘Quick Start’ screen is customizable in the associated method, and NOT modifiable from the ‘Quick Start’ screen.

If using a system with several channels, an additional option is available: Specific Channel Parameters. When this option is checked, some variables usually defined for all channels can be defined by channel. These variables are: multiplier factor, division factor, sample mass and working scale, of course as in the case of non-Specific Channel Parameters mode, internal standard values and User inputs variables remain channel dependent.

If using this option, the user must enter values in each acquisition part of the method of each channel. If not using this option, the acquisition part of the method is common to all channels (of the same injector).

This means that during acquisition (Quick Start or Sequence), different values can be entered for these variables according to the channels.

Pre-processing

Subtract a Blank to a Chromatogram

In the preprocessing section of the method, it is possible to select a blank chromatogram that will be subtracted from the sample chromatogram before any further calculation.

Press the Open icon: and select the blank chromatogram in the Open file window. If the blank chromatogram has been acquired on several channels, the channel to be subtracted must also be selected. The blank must be acquired with the same frequency (number of points per minute) than the one of the original chromatogram.

Subtracting a file of the Same Sequence:

In the sequence, it is possible to define blank files that will be subtracted from the following chromatograms to be acquired. To define a blank sample run, blank must be selected in the sample type column of the sequence.

For example if a sequence consists of ten lines: The first and sixth ones should be blank files and should be subtracted from the second to the fifth and the seventh to the tenth runs respectively. The only operation necessary is to select Blank in the Sample type column for the first and the sixth lines.

Recovering Raw Data:

When a blank is subtracted from a chromatogram, the raw data are not lost: to recover it, delete the blank called in the pre-processing section of the method with the button, and then reprocess (F6) the chromatogram and the raw data are recovered.

Integration

Integration Events

Peak Detection Events

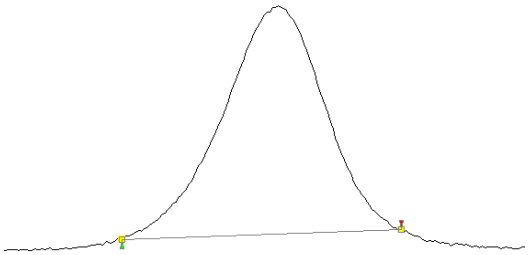
Set peak width

This event defines the width of the peak to be found in the chromatogram. This value is used to smooth the chromatogram by grouping several acquisition points during peak detection. The number of grouped points depends on the chosen width. A point whose height is the mean of all the points in the group represents each group.

Enter a value corresponding approximately to the width of the narrowest peak to be detected in the chromatogram.

If the peak width varies greatly in the same chromatogram, it is possible to change peak widths throughout the chromatogram as necessary. Set new values in Set Peak Width, half it using Half Peak Width, or double it using Double Peak Width.

If the defined peak width value is too small, the peaks will be detected, but too late.



If the defined peak width value is too large, the peaks will not be detected at all.

A peak width must be defined before integrating the chromatogram.

The default peak width is 0.2 minutes.

Set Threshold

This parameter is used to define the start and the end of peaks and eliminates the lowest signal variations due to noise or to detector signal drift.

CompassCDS allows two types of threshold calculation: relative threshold (see page62) or absolute threshold (see page62). The absolute threshold is defined in the METHOD / INTEGRATION / PARAMETERS menu, by unchecking the Use relative threshold option. Details about the way CompassCDS detects peaks are described in the “Peak start and end determination” section (see page62).

If relative threshold is used (by default), the chromatogram is first normalized to 100,000 (Highest peak of the chromatogram) in order to obtain a similar detection from one analysis to another (for example, if the injected quantity varies). If absolute threshold is used, no preliminary calculation is done. Next, the points are grouped depending on the peak width defined above. The mean height of a group of points is compared to the mean height of the following group. If the difference is higher than the threshold, the integrator marks the beginning of a peak. The position of the marker is adjusted by considering only the points. The peak will be kept only if its area and height are larger than minimum values defined by user.

The peak ends are detected in the same way using the threshold.

The value of the threshold is important. If too high of a threshold value is defined, the peak starts will be detected too late and the peak ends too early. Moreover, small peaks could not be detected at all. If a too small of a threshold value is defined, the peak starts will be detected too early, and the peak ends too late, and signal noise can be detected as peaks.

The user can define the threshold value, or CompassCDS can estimate it using Estimate threshold according to the peaks that should be detected.

It is also possible to add a value to the threshold using Add to threshold. For example, if the threshold is estimated at the beginning of the analysis, and the signal noise increases at the end of the analysis, the threshold will need to be increased only at the end. Note that it is possible to add a negative value in order to decrease the threshold value.

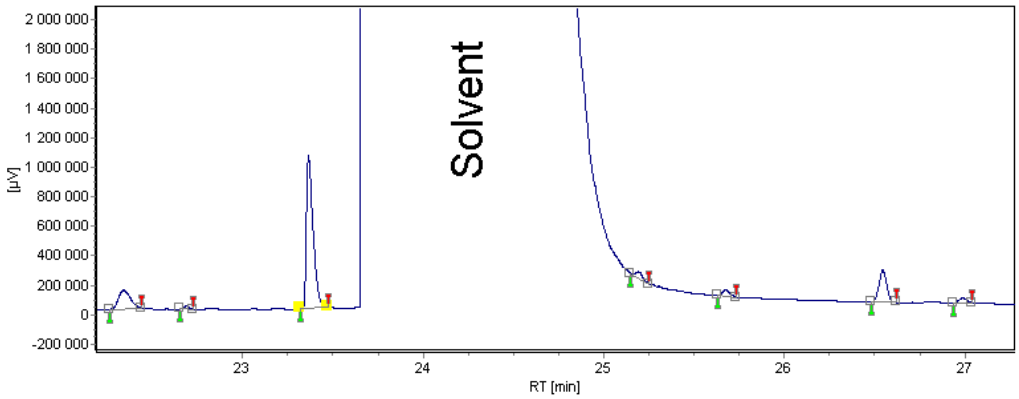
The default threshold value is 10.

Set Solvent Threshold

This event performs the elimination of solvent peak(s) if they are not peaks of interest.

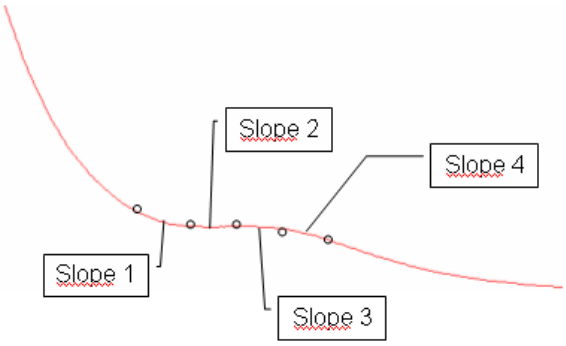
The parameter associated with this event works in a manner similar to the absolute threshold (without previous normalization of the chromatogram). The points are grouped depending on the peak width defined above. The mean height of a group is compared to the mean height of the following group. If the difference is higher than the solvent threshold, CompassCDS considers that the peak is a solvent peak, and does not integrate it.

The defined value must be high enough to prevent the deletion of peaks of interest.



Set Shoulder Threshold

This event allows the user to have a better sensibility for detecting peaks where the peak start cannot be found easily.



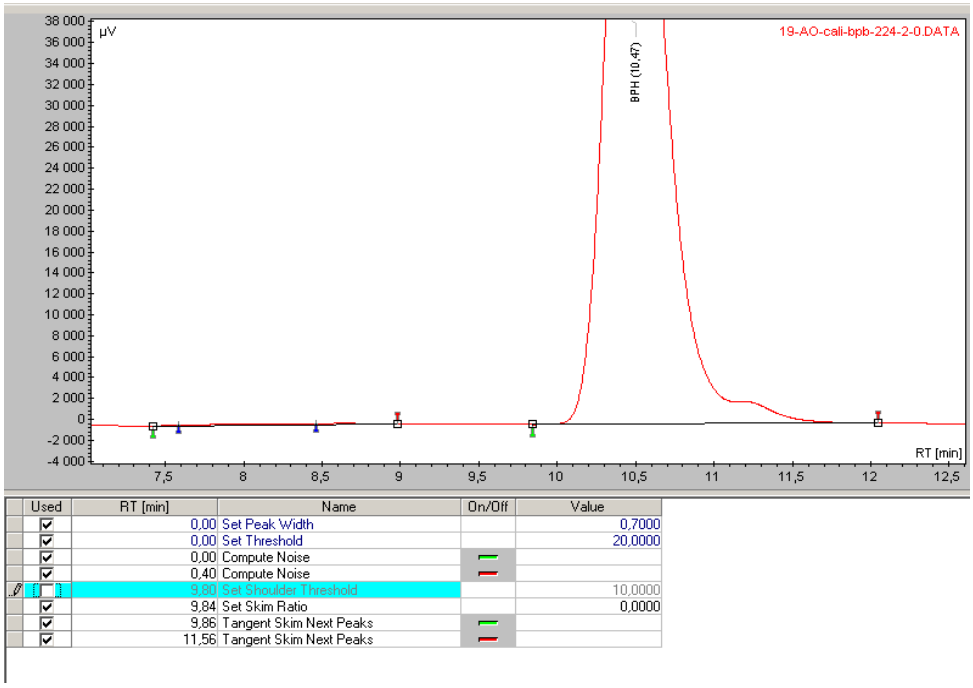
The user has to enter a value for the Shoulder Threshold event. A possible start point is determined between Slope 1 and Slope 2 when:

- |Slope 2| < Shoulder threshold
- |Slope 3| < Shoulder threshold
- |Slope 1| > Shoulder threshold
- |Slope 4| > Shoulder threshold
- Slope1×Slope4>0

NOTE: The slope is computed across the data bunch interval.

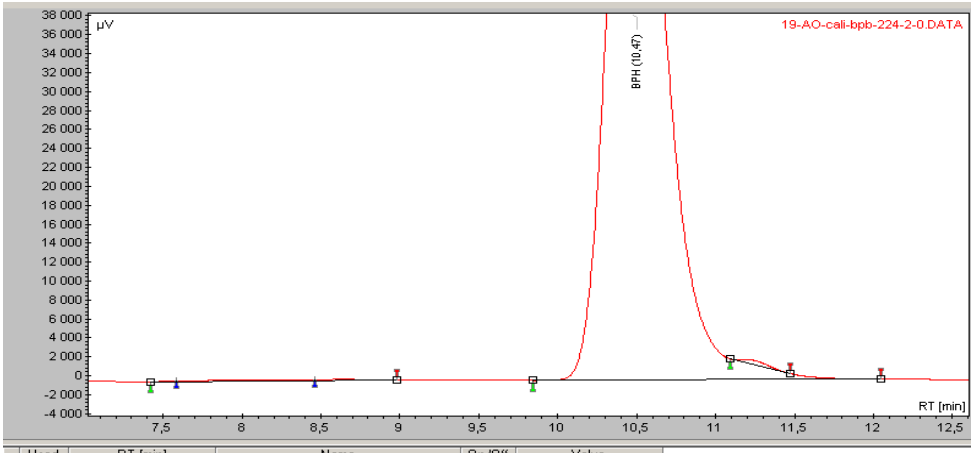
For example,

Before:



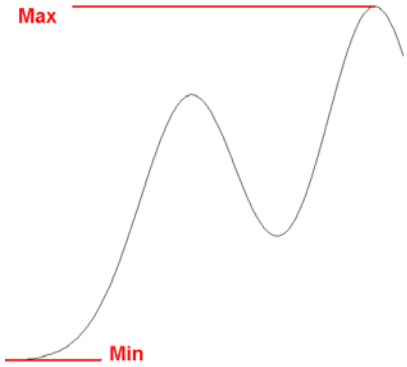
Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,7000
☑	0,00	Set Threshold		20,0000
☑	0,00	Compute Noise		
☑	0,40	Compute Noise		
☐	9,80	Set Shoulder Threshold		10,0000
☑	9,84	Set Skim Ratio		0,0000
☑	9,86	Tangent Skim Next Peaks		
☑	11,56	Tangent Skim Next Peaks		

After:



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,7000
☑	0,00	Set Threshold		20,0000
☑	0,00	Compute Noise		
☑	0,40	Compute Noise		
☑	9,80	Set Shoulder Threshold		10,0000
☑	9,84	Set Skim Ratio		0,0000
☑	9,86	Tangent Skim Next Peaks		
☑	11,56	Tangent Skim Next Peaks		

Max Y threshold %: By default to be integrated, a peak must satisfy the following condition: minimum signal value < 1% of the maximum signal value of the peak. To integrate some peaks that are not integrated by default by the software, user can reduce this value up to 0. In the contrary, to not integrate some noise on the top of a solvent peak for example, user can increase this value.



Estimate Threshold:

If the event "Estimate threshold" is not defined, solvent peaks are integrated. The user can define several events ‘Estimate threshold’. For each time the event is defined, CompassCDS calculates both absolute threshold and relative threshold (see definition in the Integration algorithm section). The calculated values are displayed in the chromatogram properties and are named: AUTOTHRESHOLD_ABS_I and AUTOTHRESHOLD_REL_I, where I represent the I^{th} defined event in the integration table.

Compute noise

This event calculates the noise value from the signal during an acquisition. (The calculations are explained in the standard global variables). The noise needs a start and an end to be calculated: Add a Compute noise ON event at the time when the noise calculation should start, then add a Compute noise OFF event at the time when it should stop. Be careful not to include peaks in the defined area because they would be considered as noise.

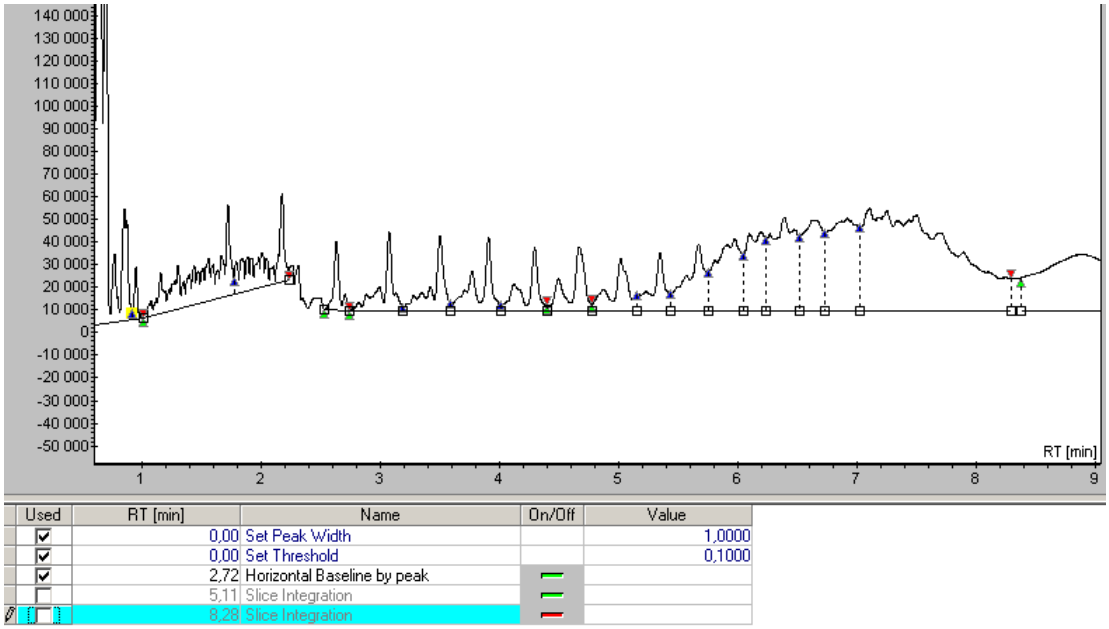
The calculated value is displayed in the chromatogram properties. The corresponding variable is "NOISE". If no time period is defined, the NOISE value is equal to 0.

NOTE: If several events (NOISE ON / NOISE OFF pairs) have been defined, only the value calculated for the last period is displayed.

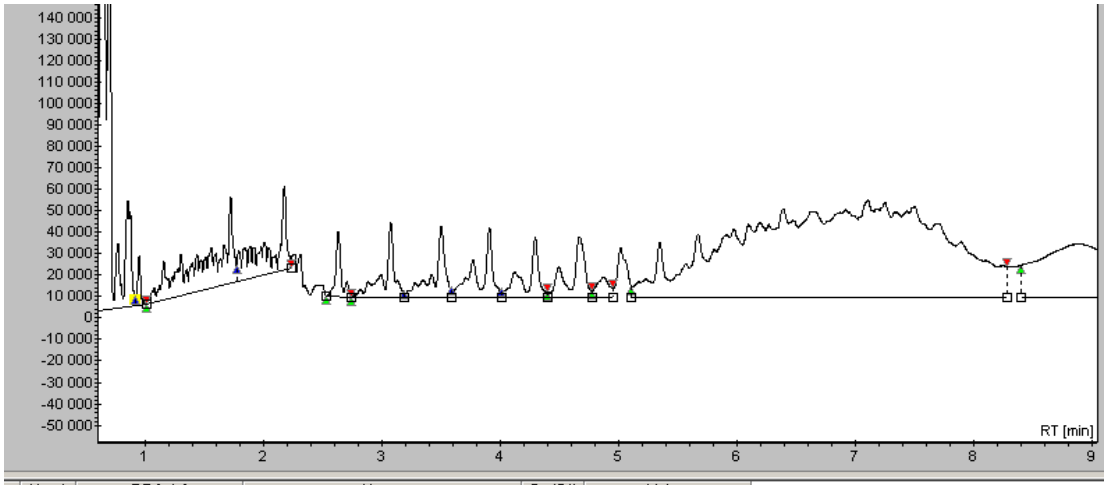
Slice integration:

This event allows the user to deactivate the automatic integration during a defined period. This can be useful to integrate a set of peaks as a single peak. This event is totally independent of the Peak width and the Set threshold.

Example:



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		1,0000
☑	0,00	Set Threshold		0,1000
☑	2,72	Horizontal Baseline by peak		
☐	5,11	Slice Integration		
☐	8,28	Slice Integration		



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		1,0000
☑	0,00	Set Threshold		0,1000
☑	2,72	Horizontal Baseline by peak		
☑	5,11	Slice Integration		
☑	8,28	Slice Integration		

Set Minimum Height/Area

These parameters are used to prevent the integration of noise as peaks or to eliminate small peaks which are not of interest in the analysis.

All peaks whose height or area is less than the minimal height and/or area parameters set are deleted from the peak report. Therefore, choose parameters that are less than the areas and heights of all the peaks to be integrated.

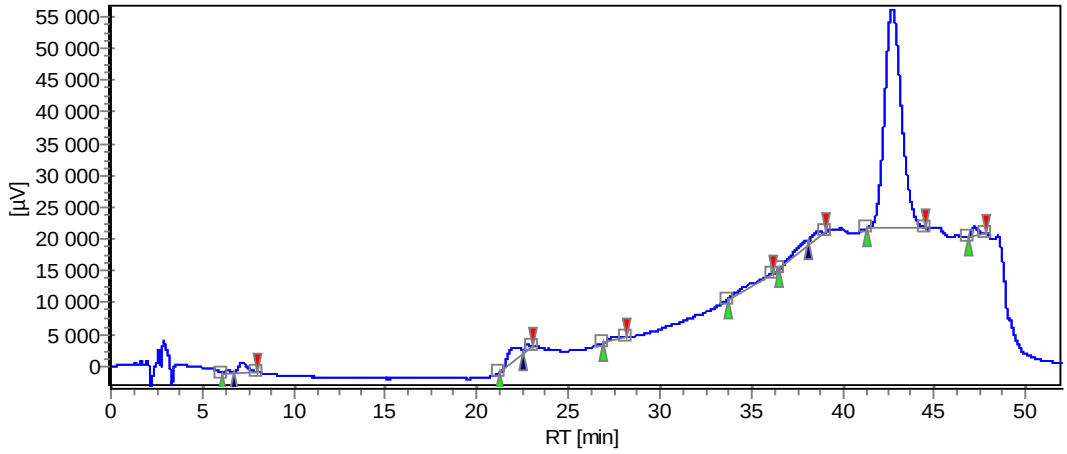
Minimal heights and areas can be defined absolutely or relatively to total chromatogram heights and areas using the events “Set minimum height %” and “Set minimum area %”.

By default, minimum area and height settings are equal to zero.

Forced peaks

Turn integration On/Off

These events activate or deactivate integration within sections of the chromatogram (e.g., during baseline fluctuations (injection shock)):



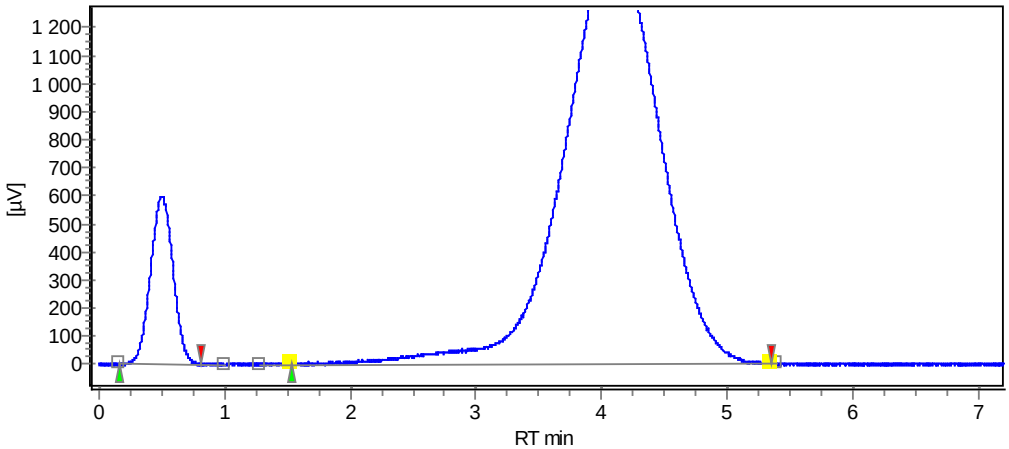
In the above example, integration has been deactivated during the first 5 minutes.

Start/Stop peak now

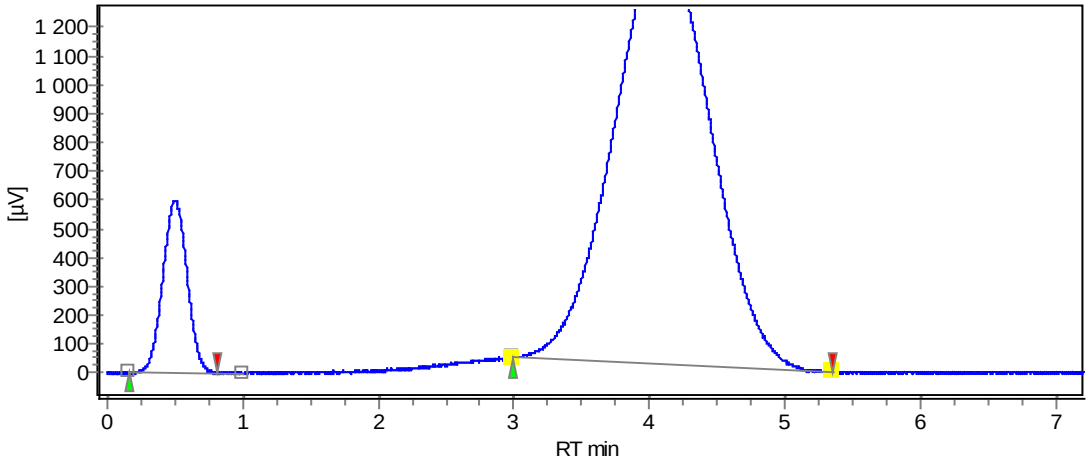
These events allow the start or the end of a peak to be defined, earlier or later, without having to modify the integration parameters. The marker is re-positioned at a new retention time when this event is specified.

For example,

Before:



After:

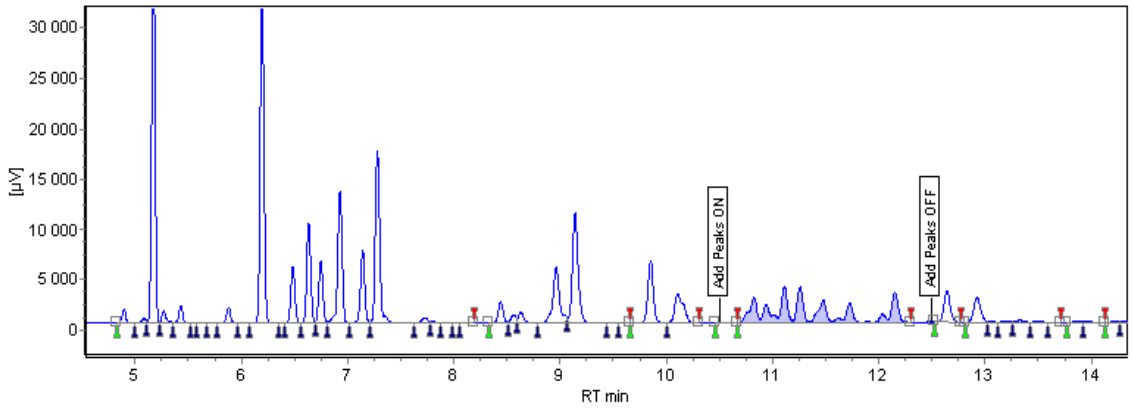


Be cautious if using these events in automatic mode: check that retention times have not shifted from one analysis to another.

Add peaks

This event enables addition of several peaks. All the peaks defined between the activation and the deactivation of this event is grouped into one peak.

For example, isomers whose names are not known peak by peak, but contain nearly the same response factors can be considered as one group. The peak grouping is considered as one peak. Note that the peak start or stop position is automatically adjusted around the defined time to avoid the baseline cut by the signal.



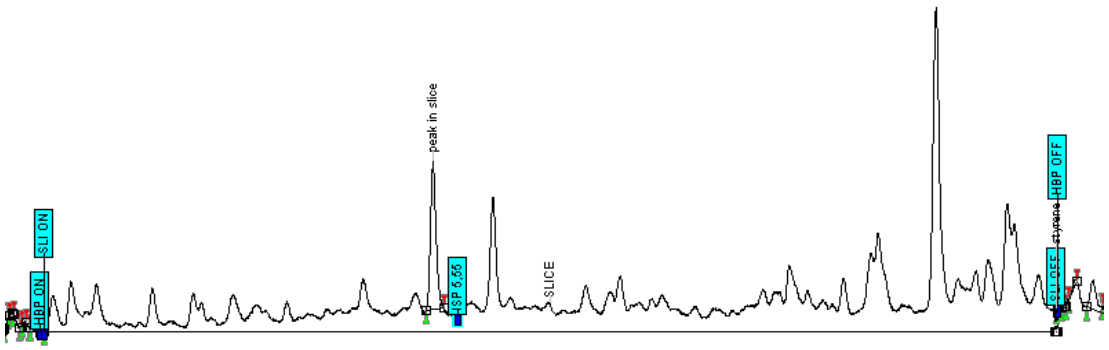
In the above example, the peaks between 10.5 and 12.5 minutes are added.

NOTE: If the baseline cuts the signal in the section corresponding to the ‘Add peaks’ events (ON + OFF), the expected added peak can be not defined. In this case, change the baseline position to the corresponding integration event(s).

In slice peak

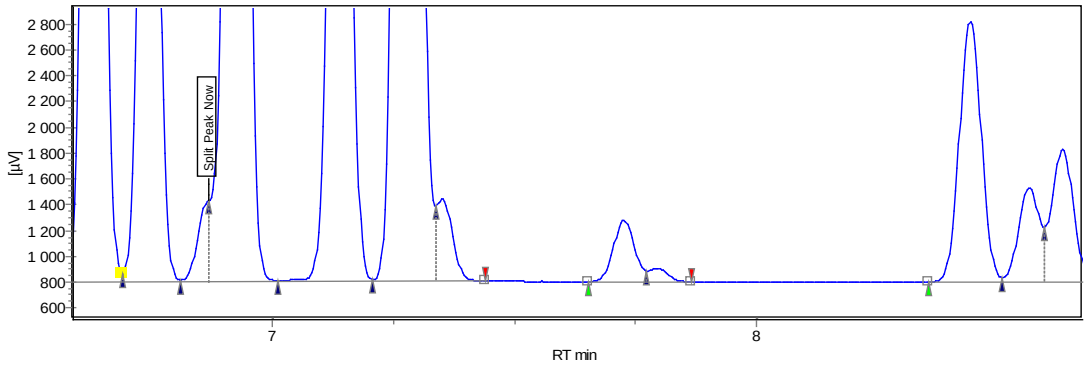
This event has to be used within a slice (between Slice integration ON and Slice Integration OFF integration events). It allows the user to add a peak in a slice. A tangential baseline is drawn between the start peak and the stop peak marker positions, and its area is removed from the slice area.

The In slice peak integration event is defined at a time with a relative windows (in minutes). The software is looking for the highest peak to integrate in the time interval defined by the user [RT± windows].



Split peak

This event will split a peak into two parts, and can be used either to separate peaks poorly resolved or to obtain specific results on parts of some peaks in certain applications.



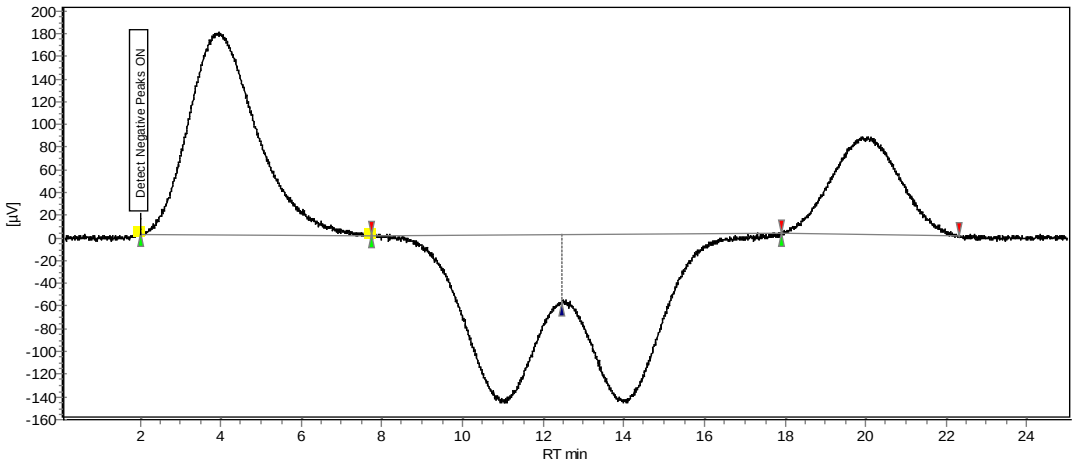
Be cautious when using this event in automatic integration mode. If retention times vary from one analysis to another the results may not be what were expected.

Negative Peaks Processing

The Detect Negative Peaks event activates negative peak detection.

When negative peak detection is activated (On), it is better to also deactivate it, (Detect negative peaks off), because during the integration algorithm the CompassCDS tries to place a baseline between these two events (On and Off). If the signal passes below this raw baseline, CompassCDS searches for negative peaks. When the signal is above this raw baseline, CompassCDS searches for positive peaks.

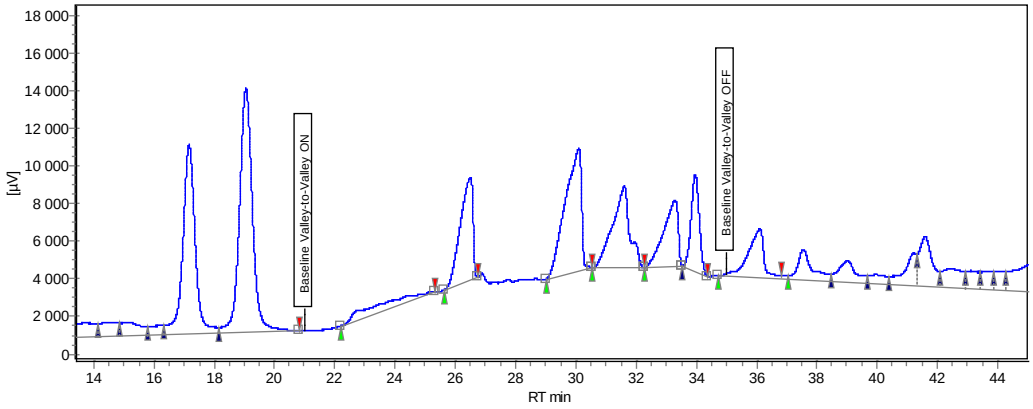
Negative peak detection depends on the signal height when the event is activated and deactivated, so it is also dependent upon the time when the events are specified. As a consequence, be careful to ensure that negative peak detection is not activated or deactivated after the beginning of a peak.



Baseline Processing

Baseline valley to valley On/Off

When this event is activated, the baseline passes through all the valleys.



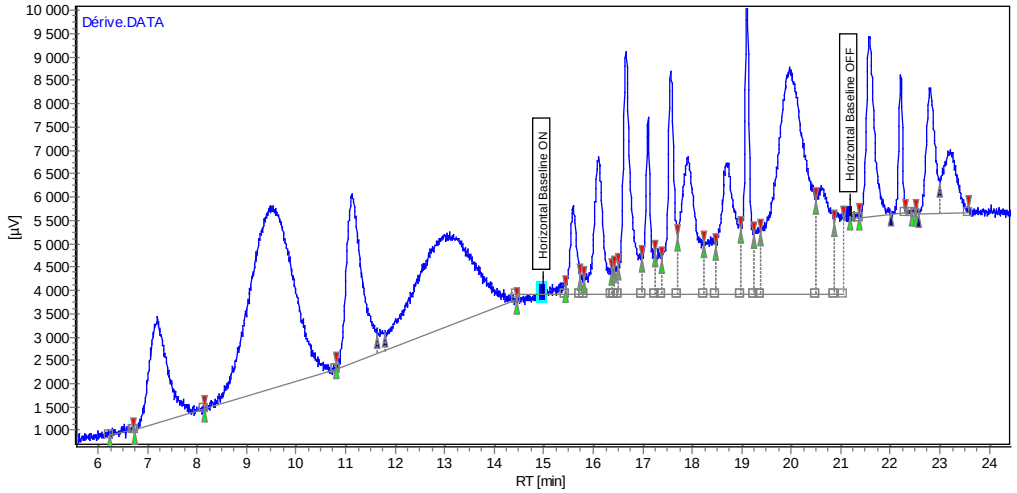
Each peak has its own baseline drawn from the peak start marker to the peak end marker.

Horizontal baseline

This event enables the definition of a horizontal baseline.

A horizontal baseline is drawn from the activation of this event until its deactivation. It is imperative to define the event couple (ON and OFF) to apply this event.

NOTE: ON is symbolized by a green mark and OFF by a red one.

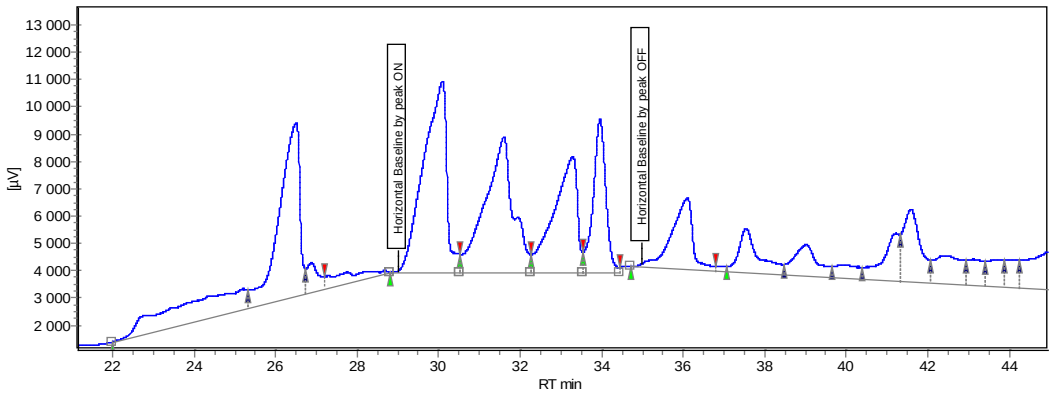


The height of the baseline is the height of the signal when the event is activated.

It is better to use the “Horizontal baseline by peak” event, because the height of the baseline will be related to the start or the end of a peak, and not to the event activation time.

Horizontal baseline by peak

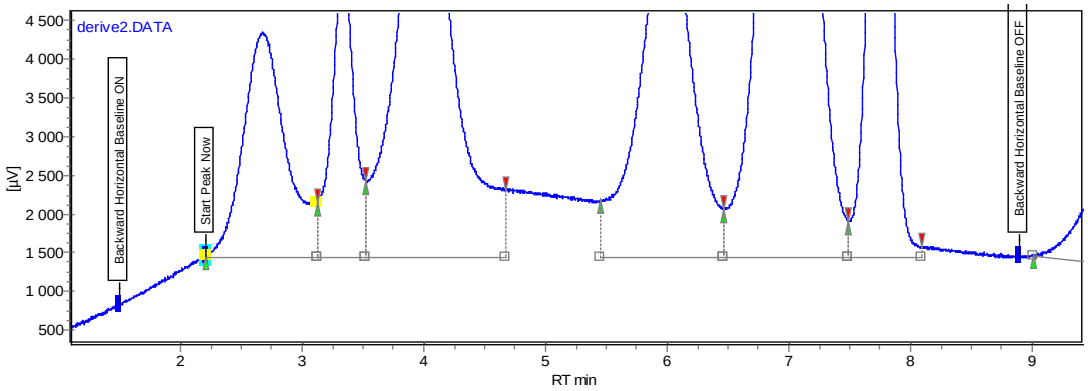
This event enables definition of a horizontal baseline. The horizontal baseline start or stop are not applied to the defined times, but to the nearest start or stop peak time



If an event is activated at the beginning of a peak (between the start marker and the peak apex), it becomes operative at the peak start time. If the event is activated at the end of the peak (between the top of the peak and the stop marker), it becomes operative at the peak stop marker time.

Backward Horizontal baseline

This event enables definition of a horizontal baseline at the level of the signal when this event is deactivated.

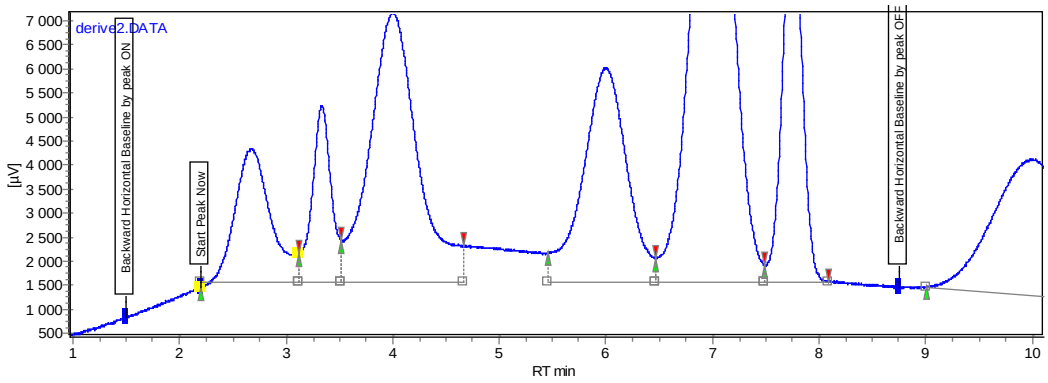


The horizontal baseline is drawn from the activation of the event until its deactivation. The baseline is drawn at the level of the signal when the event is deactivated.

As a consequence, the two events “Horizontal baseline Backward On” and “Horizontal baseline Backward Off” must be defined.

Backward Horizontal baseline by peak

This event enables definition of a backward horizontal baseline. The horizontal baseline is drawn from the activation of the event until its deactivation. The baseline is drawn at the level of the signal at the stop marker of the peak preceding the event deactivation.

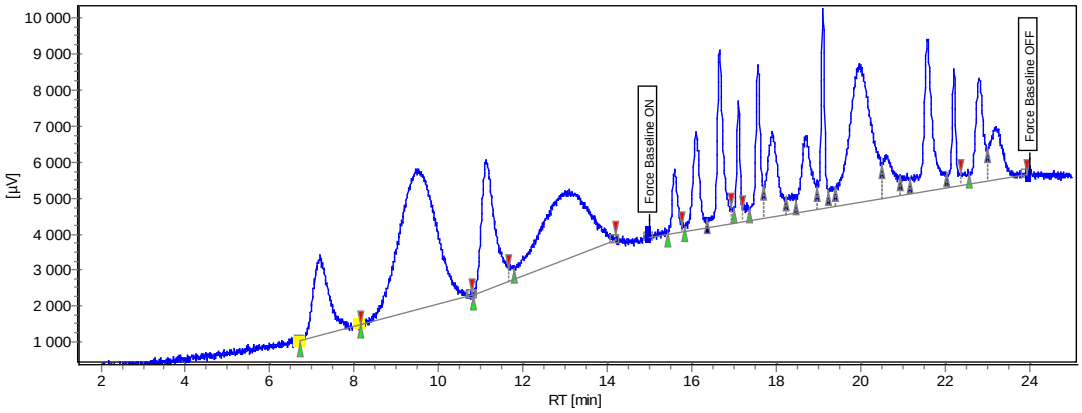


As a consequence, the two events “Backward Horizontal Baseline by peak On” and “Backward Horizontal Baseline by peak Off” must be defined.

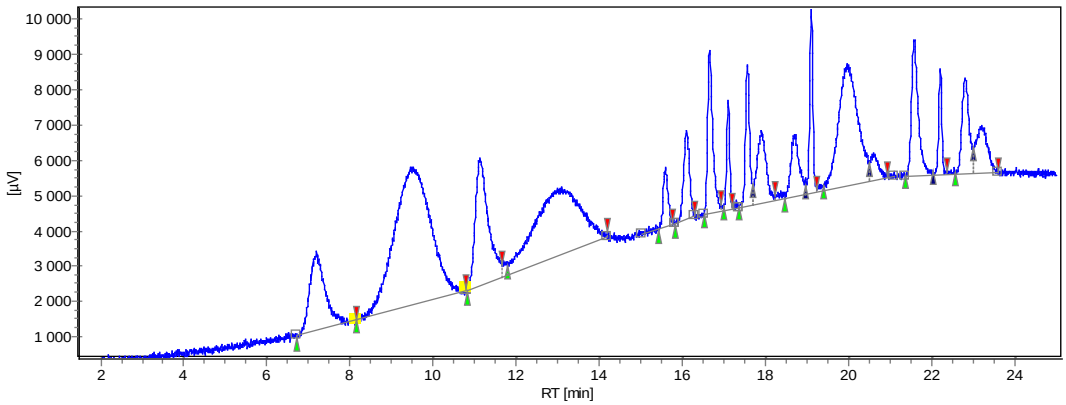
Force baseline

This event forces all the peaks between the events “Force baseline on” and “Force baseline off” to have a common baseline. The peak markers of the first and last peaks are therefore modified by this event. To prevent modification of the first and last peak markers, the recommended event to use is “Force baseline by peak”.

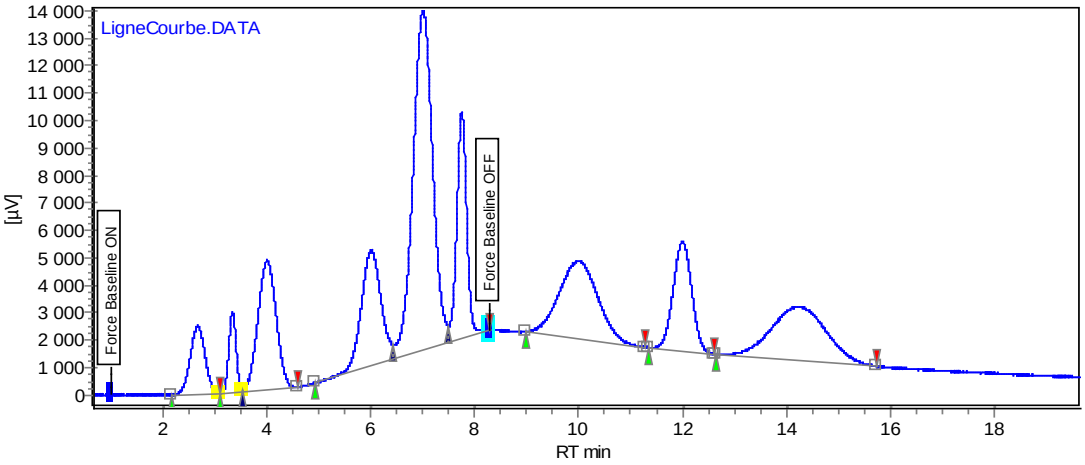
As a consequence, the two associated events “Force baseline on” and “Force baseline off” must be defined.



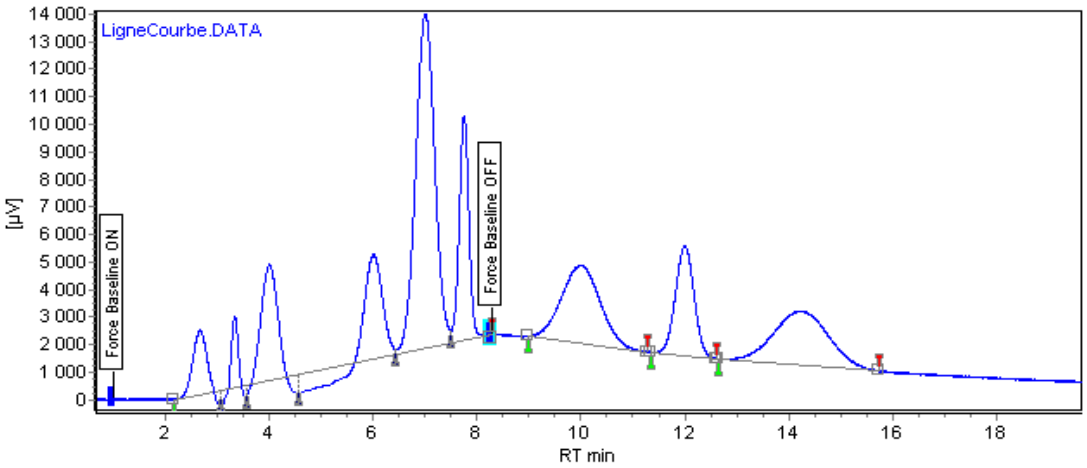
Instead of



If the forced baseline penetrates the signal, the baseline will automatically adjust so that it always remains under the signal.



Instead of



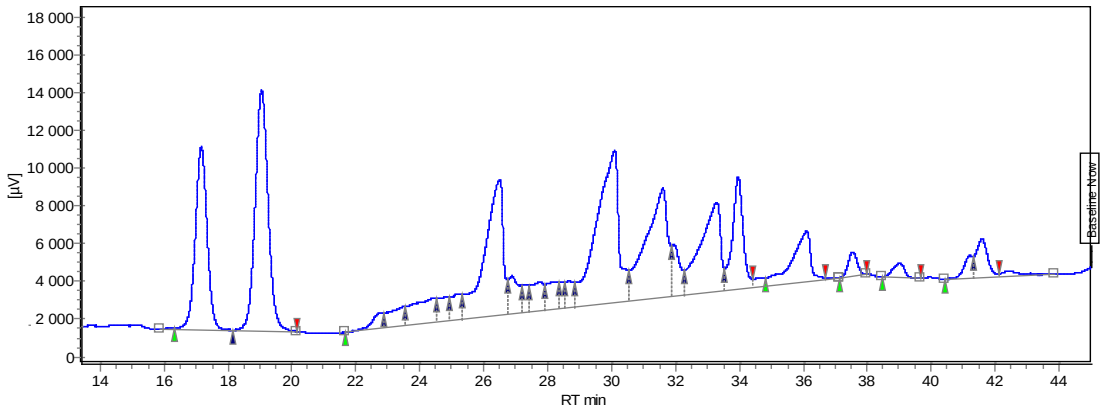
Force baseline by peak

This event forces all the peaks between the events “Force baseline by peak on” and “Force baseline by peak Off” to have a common baseline.

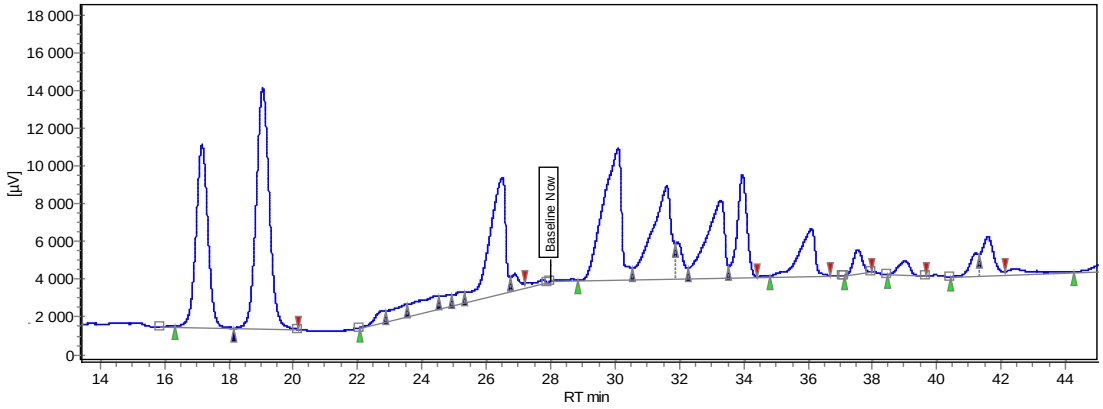
The difference with force baseline is that in this case, the markers of the first and the last peak are not modified.

Baseline now

This event forces the baseline to pass through the signal at the event time.



Becomes



This event is used to

- Bring the baseline back to the signal.
- Separate peaks which have a common baseline.
- End earlier a tailing peak.

The position of this event is relative to retention time drift, but as for most of the events, a similar peak-dependent event exists: “Baseline next valley”.

Baseline next valley

This event is similar to the previous one (Baseline now). The only difference is that CompassCDS waits for the valley following the event to bring back the baseline to the signal.

As a consequence, this event is best suited for separation of peaks having a common baseline, since “Baseline next valley” is less dependent on retention time variations from one analysis to another.

Shoulder Peaks:

To integrate a peak as the skimming of another, both peaks need first to be integrated. Thus it is important to define correct detection parameters (Set peak width and Set threshold) before defining the skimming parameters.

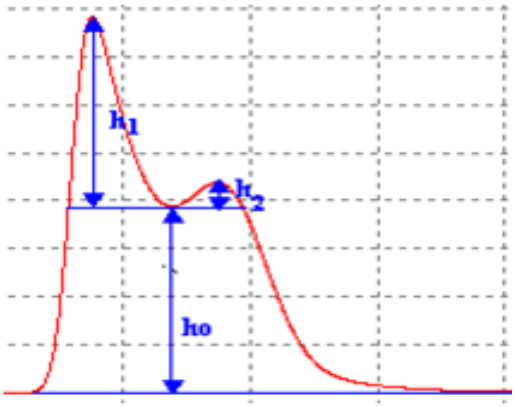
Set skim ratio

This event allows the user to set the shoulder integration threshold above a mother peak. This threshold must be associated to the events “Tangent skim front/rear” and “Exponential skim front/rear”.

A peak will be integrated as a shoulder peak on another peak, if its height satisfies the shoulder peak criterion.

In the following example, the second peak will be considered as a shoulder on the first peak if:

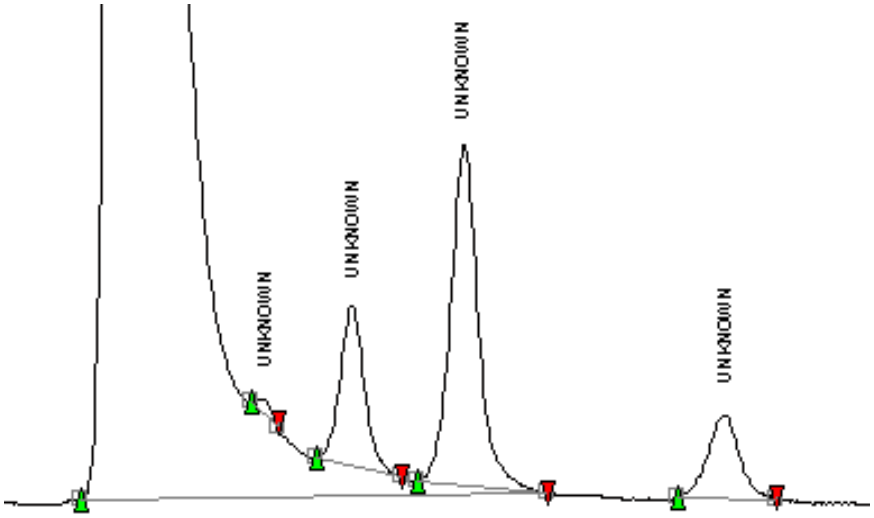
$$\frac{h_1}{h_2} \geq \text{parameter} \quad \text{and (ho} \neq 0)$$



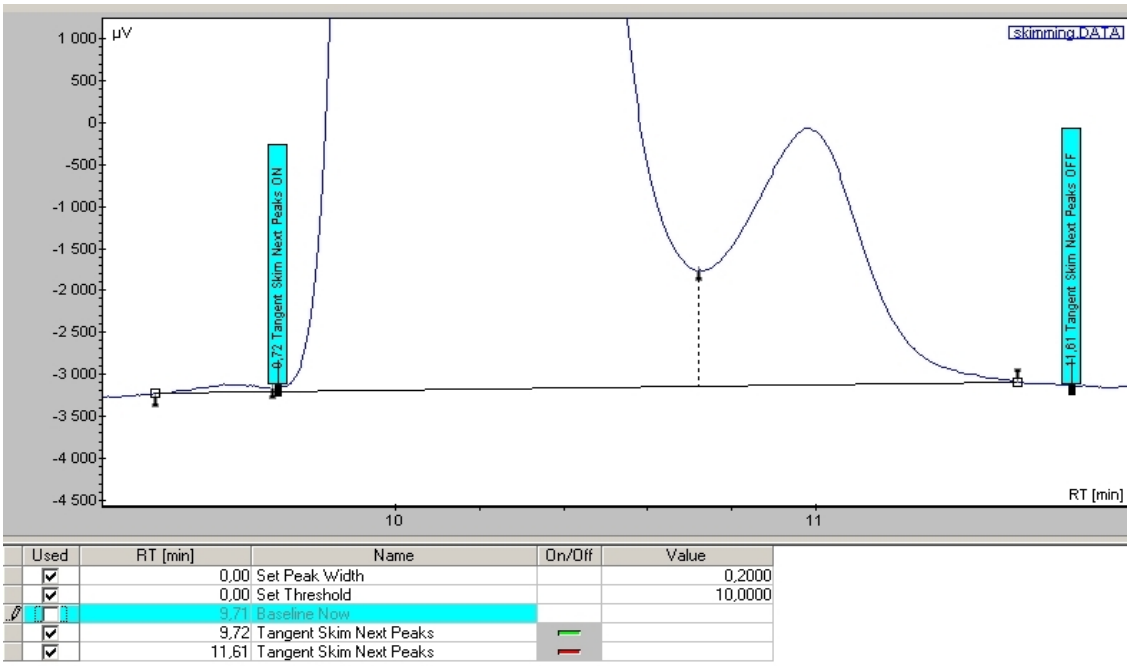
By default, this threshold is equal to 4.

Tangent skim next peaks On/Off

If this event is activated (On), all the peaks having a common baseline are integrated as shoulder peaks on the first peak, with a tangent baseline.

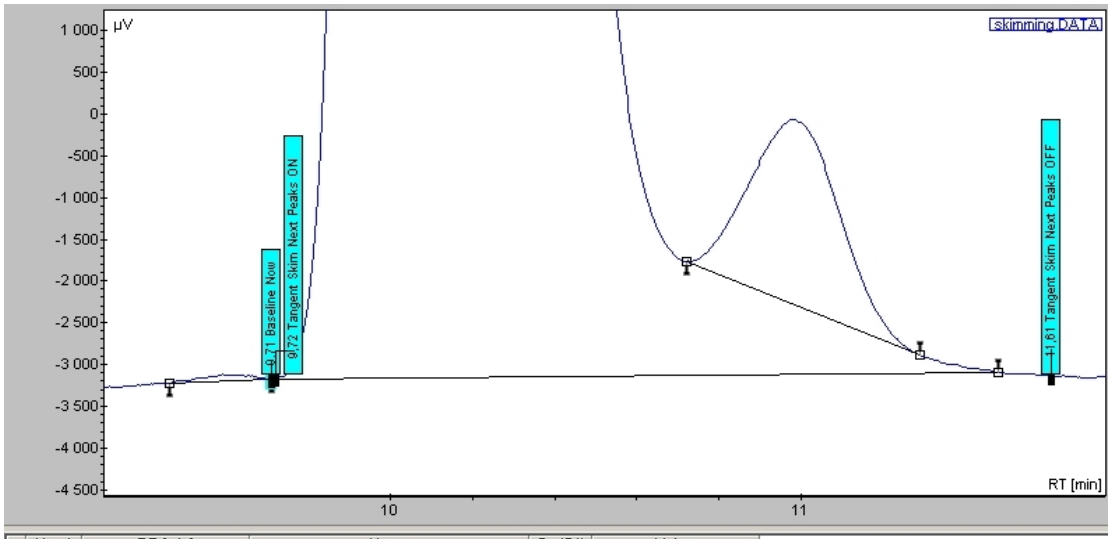


The tangent skim Next Peaks event does not work when the mother peak is not fully resolved (e.g., has a valley with the previous peak). The use of a Baseline Now event has the effect of removing the valley, and thus allows the skimming event to work properly. See figures below.



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,2000
☑	0,00	Set Threshold		10,0000
☐	9,71	Baseline Now		
☑	9,72	Tangent Skim Next Peaks		
☑	11,61	Tangent Skim Next Peaks		

Without the baseline now event, there is a group of three peaks sharing a common baseline



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,2000
☑	0,00	Set Threshold		10,0000
☑	9,71	Baseline Now		
☑	9,72	Tangent Skim Next Peaks		
☑	11,61	Tangent Skim Next Peaks		

The baseline now event just breaks the group of peaks

Note that there is another event, more powerful, called Tangent Skim Rear, which handles such situations.

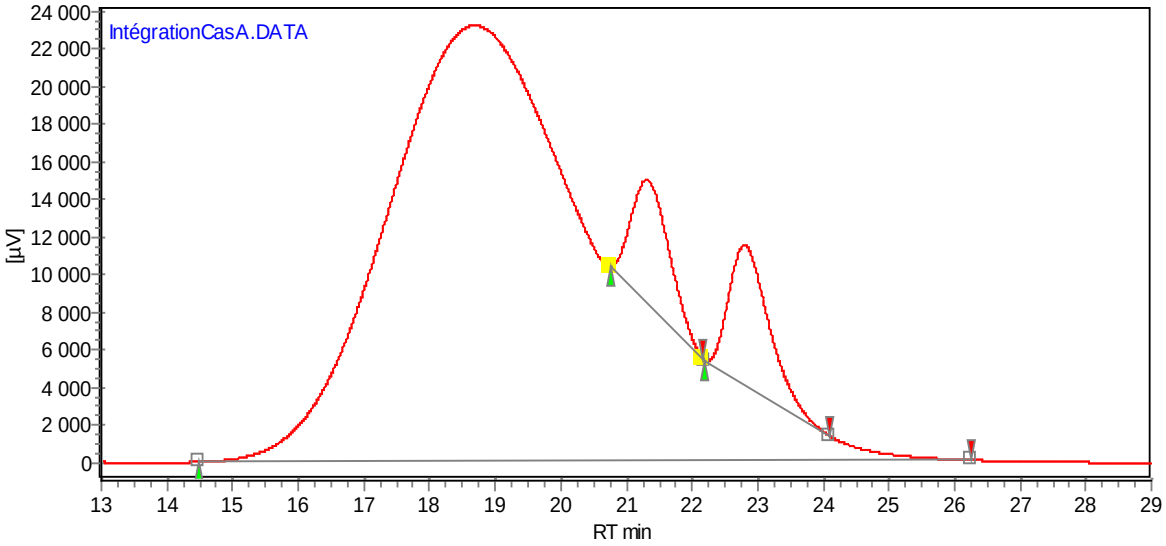
Exponential Skim Next Peaks On/Off

If this event is activated (On), all the peaks having a common baseline are integrated as shoulder peaks on the first peak, with an exponential baseline.

Tangent skims Rear/Front

Select this event to integrate one or several peaks as shoulders on a mother peak with a tangent baseline.

If CompassCDS detects poorly resolved peaks whose heights satisfy the above height criterion (see page 57), a tangent baseline is drawn underneath the shoulder peaks.

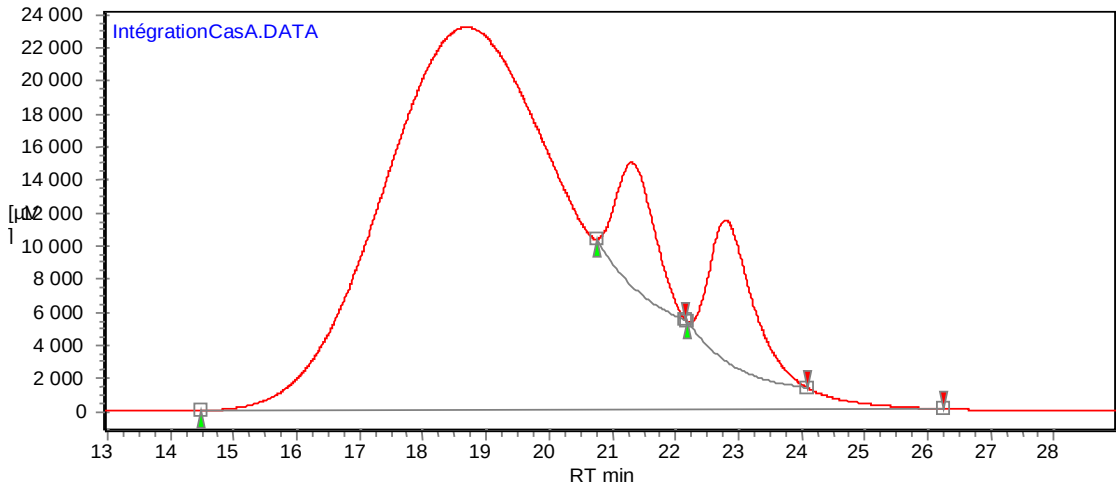


If the event is “Tangent skim front”, the shoulders are integrated before the mother peak. If the event is “Tangent skim rear”, the shoulders are integrated after the mother peak.

Exponential skim rear/front

Select this event to integrate one or several shoulder peaks with an exponential baseline.

If CompassCDS detects two poorly resolved peaks whose heights satisfy the above height criterion (see page 57), an exponential baseline is drawn underneath the shoulder peaks.



NOTE: The popup menu of the integration event table contains a Copy option that enables to copy the list of events before to paste it into another application.

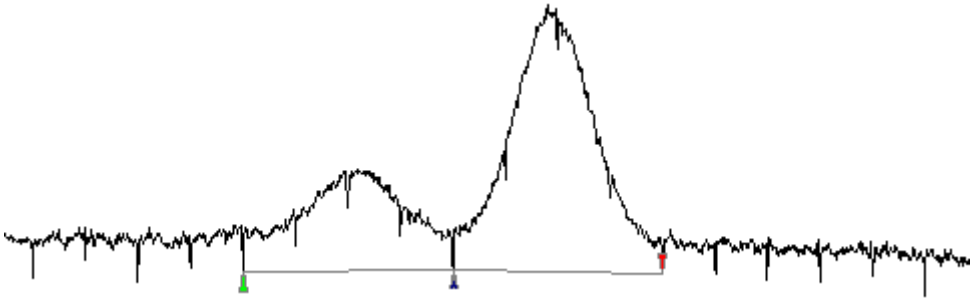
Integration Algorithm:

The integration algorithm operates in 4 stages: Spike reduction, data bunching, peak detection and baseline construction.

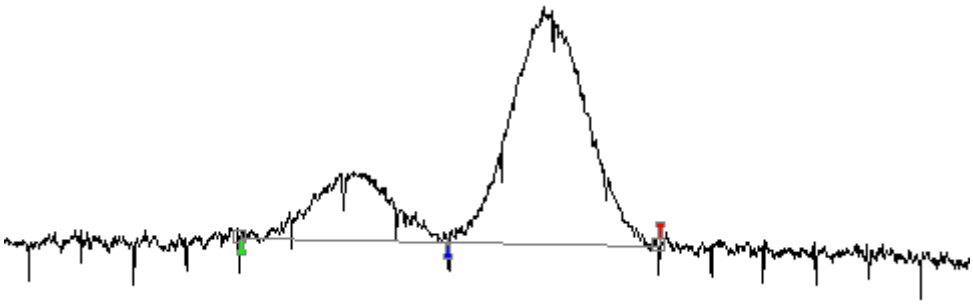
Spike Reduction

This stage is very useful if the signal is perturbed, and particularly with negative spikes. This stage can also be used to filter a part of the noise (and especially cyclic noise).

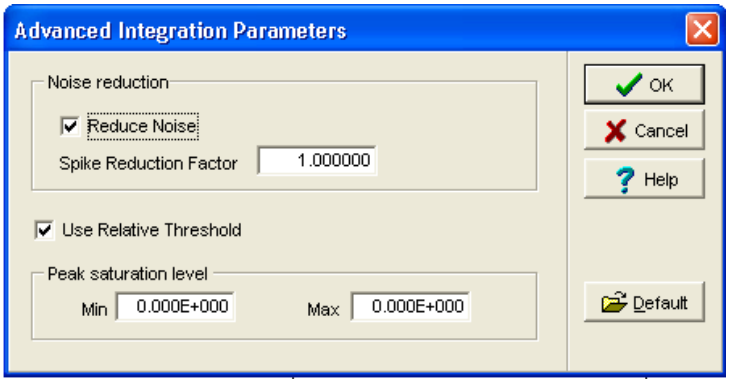
In the following example, some spikes perturb the chromatogram; the baseline is placed between the lowest points (the bottom of the spikes). Thus the area calculations are wrong:



If the spike reduction is activated, the spikes will be eliminated from the signal and the baseline drawn on this signal:



This step can of course be bypassed and the parameters defining the strength of the spike reduction can be modified. These parameters are defined in the advanced integration parameters, available using the METHOD / INTEGRATION / PARAMETERS menu:



Uncheck the Reduce noise box to deactivate the spike reduction.

Change the spike reduction factor to modify the way .is eliminated. The larger the spike reduction factor is the more noise will be eliminated. A value of Ø corresponds to no reduction. A value of 1 (default value) is generally a good compromise. In the above example, the specified value was 5. Be careful a too high value could eliminate small peaks.

Data Bunching

After the spike reduction, the chromatogram points are bunched and the peak starts and stops are detected. This step will eliminate some additional noise (random noise).

During data point bunching, the chromatogram is examined and every n point group is averaged into one point. Then the peak start and end determination is done with these bunched points.

Data bunching uses mean points in order to improve the peak start and end determination. The number of points that are bunched depends on the peak width defined in the integration method:

$$n = \frac{W}{15 \times \Delta t}$$

W is the peak width (in minutes) set in the integration method.

Δt is the acquisition period (inverse of the acquisition frequency), i.e., the time interval between two acquisition points (in minutes). This global variable is called DELTAT in the CompassCDS Chromatography Data System software.

A peak should contain at least 15 bunched points to be well detected.

Peak Start and End Determination

The peak starts and ends are determined using the bunched data points and the threshold entered in the integration method.

CompassCDS allows the integration of a chromatogram with two threshold types: normalized threshold (used by default) or absolute threshold.

Normalized Threshold

The threshold is “normalized” in order to reduce the influence of the injected amount:

$$Th_{norm} = Th \times \frac{Y_{max}}{100{,}000}$$

Th_{norm} is the normalized threshold

Th is the threshold entered in the integration method

Y_{max} is the maximum value of the signal along the chromatogram

Then, to determine peak starts and peak ends, the variation of the height between the bunched data is compared to the normalized threshold:

First of all, a peak start is searched:

If P1 is the height of a point, it is compared to P2, the height of the next point and P3, the height of the second next point:

Calling h1= P2-P1 and h2= P3-P2,

If h1> Th_{norm} and h2> Th_{norm} and if $\frac{h1+h2}{2}$ > Th_{norm} then a peak start is created in P1.

Then a peak apex is searched:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a peak apex is detected in P1.

After a peak apex, valleys or peak ends are searched:

Valley:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a valley is created in P1.

Note that the test is the same as for a peak apex, but after a peak apex if this test is positive, it means that there is a valley.

Peak end:

If P1 is the height of a point, it is compared to P2, the height of the previous point, P3, the height of the second previous point and P0 the height of the next point:

Calling h1= P2-P1, h2= P3-P2 and h3=P1-P0

If h1< Th_{norm} , h2< Th_{norm} and h3< Th_{norm} then a peak end is created in P1.

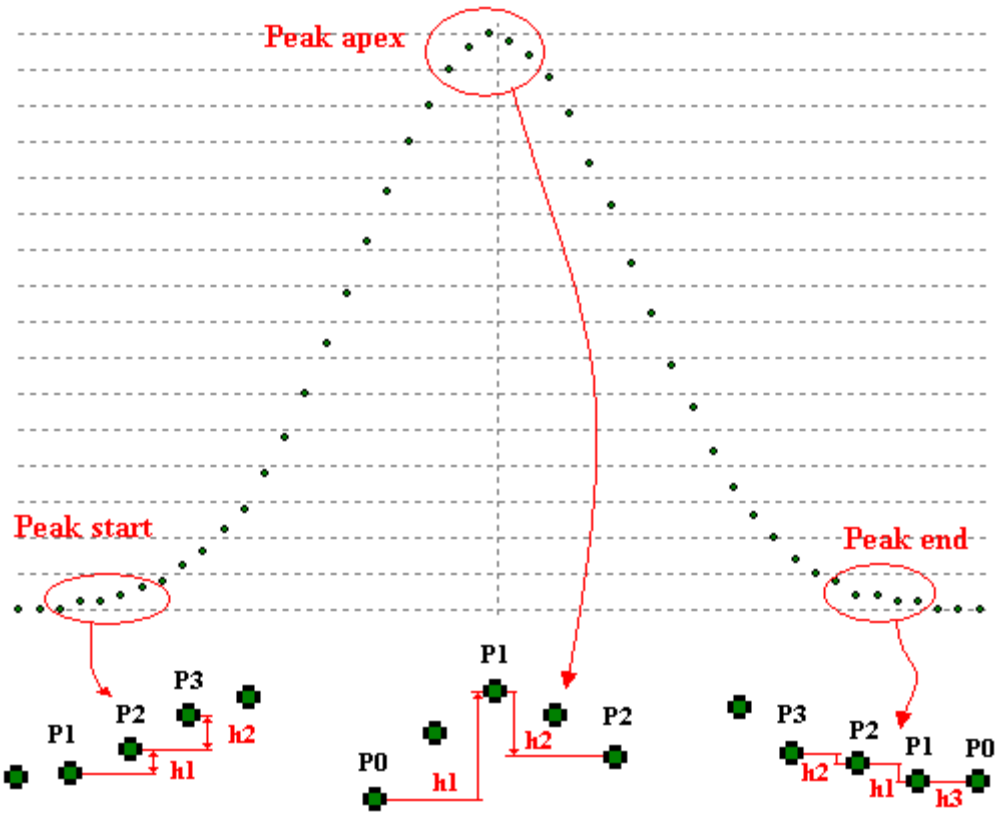
A peak apex is searched after a valley whereas a peak start is searched after a peak stop.

If negative peak detection is activated, the succession of peak starts, apexes, valleys and ends are the same, the test for peak apexes and valleys is the same as define above, the test for peak start and end is the opposite:

If h1<- Th_{norm} and h2<- Th_{norm} and if $\frac{h1+h2}{2}$ <- Th_{norm} then a peak start is created in P1.

If h1>- Th_{norm} , h2>- Th_{norm} and h3>- Th_{norm} then a peak end is created in P1.

Here are the ways the peak ends and apex are determined:

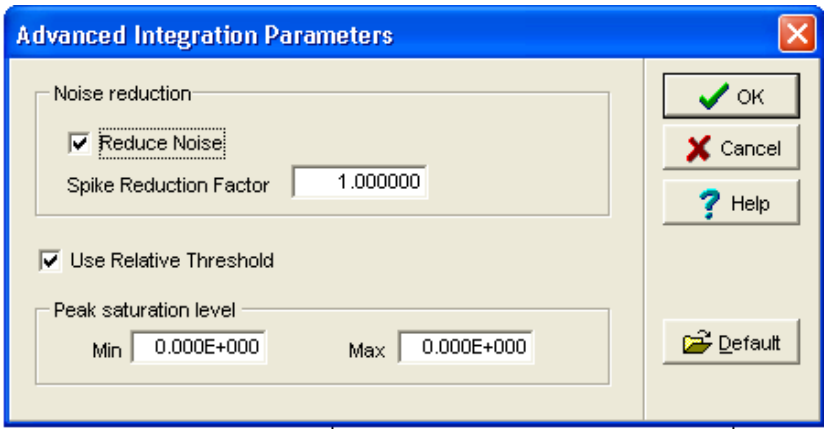


Afterwards the position of the marker is adjusted by considering only the points. The peak will be kept only if its area and height are larger than minimum values.

Absolute Threshold

In some analyses, the major peak size (solvent for example) changes a lot. If the normalization is made on the maximum height peak, this can modify the integration of the other peaks of the chromatogram. In these cases, it is advised to define an absolute threshold: select the METHOD / INTEGRATION / PARAMETERS menu.

The following screen is displayed:



Uncheck the Use relative threshold option.

Then CompassCDS defines the start and end of peaks.

First of all, a peak start is searched:

If P1 is the height of a point, it is compared to P2, the height of the next point and P3, the height of the second next point:

Calling h1= P2-P1 and h2= P3-P2,

If h1> Th and h2> Th and if $\frac{h1+h2}{2} > Th$ then a peak start is created in P1.

Then a peak apex is searched:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a peak apex is detected in P1.

After a peak apex, valleys or peak ends are searched:

Valley:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a valley is created in P1.

Note that the test is the same as for a peak apex, but after a peak apex if this test is positive, it means that there is a valley.

Peak end:

If P1 is the height of a point, it is compared to P2, the height of the previous point, P3, the height of the second previous point and P0 the height of the next point:

Calling h1= P2-P1, h2= P3-P2 and h3=P1-P0

If h1< Th , h2< Th and h3< Th then a peak end is created in P1.

A peak apex is searched after a valley whereas a peak start is searched after a peak stop.

If negative peak detection is activated, the succession of peak starts, apexes, valleys and ends are the same, the test for peak apexes and valleys is the same as define above, the test for peak start and end is the opposite:

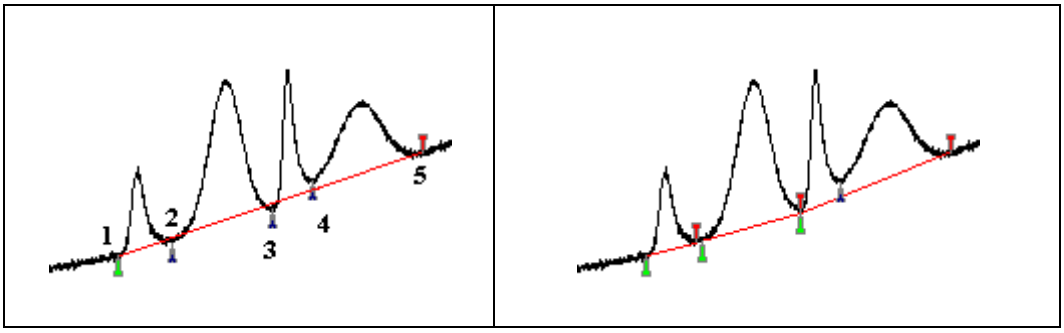
If h1<- Th and h2<- Th and if $\frac{h1+h2}{2} < -Th$ then a peak start is created in P1.

If h1>- Th , h2>- Th and h3>- Th then a peak end is created in P1.

Baseline Construction

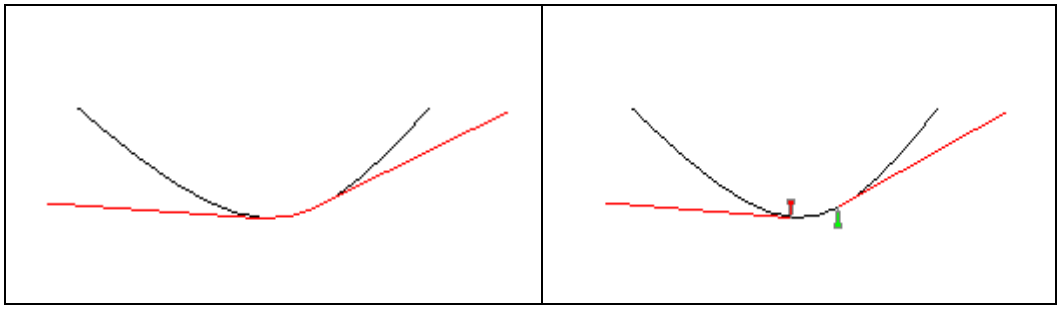
Where the peak starts and ends are defined, the baseline must be constructed:

A baseline is drawn between a peak start and the next peak end. The algorithm then checks that the baseline does not cross the chromatogram signal. If it does and negative peak detection is not activated, the baseline is modified by applying the tangent method in order not to intersect the signal.



Becomes

In the above example the baseline intersects the signal at points 2 and 3. Therefore the baseline is modified: it is drawn, as if it is a rubber band between the first peak start (1) and the last peak end (5). At points 2 and 3 the rubber band moves to follow the signal, e.g., when the baseline first touches the signal at 2 a peak end is generated and when it moves away from the signal, a new peak start is generated.



Peak Identification

This stage is used to identify peaks present in a chromatogram.

The Peak Identification Table

The first step is to fill out the identification table.

The identification table associates a peak, identified by its retention time to a name. It is possible to define reference peaks by checking the Reference peaks box. These are then used for the peak identification when differences in the retention times due to analytical conditions, occur.

How to build an identification table

To fill a table, press the right mouse button when in the table and a popup menu will appear.

Using the ADD menu option, insert as many lines as needed, then fill in the retention times and the names.

If the chromatogram has already been integrated, the identification table can be filled automatically with the retention times of all the peaks integrated in the chromatogram or peak(s) can be added one by one in the table.

First integrate the chromatogram by using either the icon, the F5 key, or by selecting the PROCESSING / INTEGRATE menu. Then,

- To list all the integrated peaks in the table, select the peak identification chromatogram method subsection and click within the peak identification page to access the popup menu, choose the INITIALIZE FROM CHROMATOGRAM option. CompassCDS will then paste the retention times and names for peaks (UNKNOWN-I) contained in the chromatogram (if any).
- To list only peaks of interest in the identification table, select the peaks one by one in the chromatogram picture, then select the Peak / Add to peak ID table option in the context menu. A line is automatically added in the peak identification table, the peak is temporarily named UNKNOWN-I, and its retention time is listed. The user will then be able to modify then name and the identification windows if needed.

Each line of the table represents one peak. In each line, enter the name of the compound corresponding to the peak, identified by its retention time and then choose the identification window width in the columns “Abs. Windows” and “Window percentages” and the identification mode.

It is also possible to fill the peak identification table from Excel. First define the peak names and RT in Excel (in columns and in this order), copy those parameters, and then select the ‘Initialize from clipboard’ option, available from the peak identification table context menu. The table is automatically filled The user can also copy an identification table, by using the ‘Copy’ option of the peak identification table context menu and paste it in Excel, then import the table in another method.

NOTE: Only the peak names and the retention times are imported from Excel in the identification table.

To delete an identification table line, highlight it by left clicking at the beginning of the line that is to be removed, then right click and choose DELETE CURRENT in the popup menu. To delete several lines, select them by left clicking in the first empty column of the table and drag the mouse to select several lines, and/or using the Ctrl and Shift keys as in any Windows application. Right click within the table to access the popup menu, then choose the DELETE SELECTION option. It is also possible to delete the entire identification table by choosing DELETE ALL in the popup menu.

The popup menu of the peak identification table contains a Copy option that enables its content to be copied and pasted into another application.

Identification table columns

Peak Name: The name of the compound corresponding to the peak. Two different peaks cannot have the same name.

Retention Time: The theoretical retention time of the peak. Two different peaks cannot have the same retention time.

Abs. Window: The absolute part of the identification window.

Window %: The relative part of the identification window.

These windows define the maximum interval around the retention time in which the peak will be assigned a specific compound name.

The absolute identification window is defined in minutes and in 1/100 of minutes. The relative identification window is defined as a percentage of retention time. If the relative identification

window percentage (Window %) is used, the larger the retention time is, then the wider the relative retention time window will be.

If retention time is RT, absolute window is Abs, and relative window is %W, a peak will be identified as the peak if its retention time is between

$$RT - Abs - \left(\frac{\%W \times RT}{100}\right) \text{ and}$$

$$RT + Abs + \left(\frac{\%W \times RT}{100}\right)$$

The identification window can thus be defined in minutes using absolute or relative windows, or defined using a combination of both.

The reference peak identification windows are treated separately. The reference peaks are identified first followed by all other peaks. If the reference peaks are correctly identified in these windows, it is possible to then define larger windows for reference peaks. This will ensure that they will be found, even if a retention time offset occurs.

NOTE: To display the identification windows, select the peak in the identification table and select the icon. If the retention time of the peak is recalculated according to reference peak(s), the window is centered on the recalculated time.

Cal.: This column selects which peaks are to be calibrated. There is a link between the identification and the calibration tables: each peak whose Cal. box is checked is added automatically in the calibration table.

Ref: This column appears only if the reference Mode is selected, which is indicated by the checked Reference peaks box.

To select reference peaks, check the Ref? box in the appropriate line(s) to indicate that the selected peak is now considered a reference peak. The theoretical retention times of the peaks will be corrected according to the difference between theoretical and experimental retention time of these peaks (see Non-reference peaks expected retention time).

The reference peaks must be chosen carefully. Reference peaks must be common constituents that will always appear in the chromatogram. If a reference peak is not present, another peak could be incorrectly assigned as the reference peak, and thus, the identification of the other peaks will be severely affected. Reference peaks should be easily recognizable. It is better to choose very high or large peaks or the last peak of the run (with the certainty that no other peak will occur afterward).

Mode: This column defines which peak will be chosen if several peaks are included in the identification window.

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the identification window.

Last: The peak will be the last peak found in the identification window.

Peaks are always listed in the retention time order.

Identification Process

Peaks are identified by their retention times, according to the identification window defined by user. In simple cases, peaks retention times are reproducible from one analysis to the other. In the case of non-reproducible retention times from one chromatogram to the other (due to analysis conditions, samples etc.), identification is more complicated and the definition of easily identifiable reference peaks is advisable. CompassCDS will identify in a first step the reference peaks and will estimate the time offset (according to the retention time) that will be applied during the identification of the other peaks of the chromatogram (non-reference).

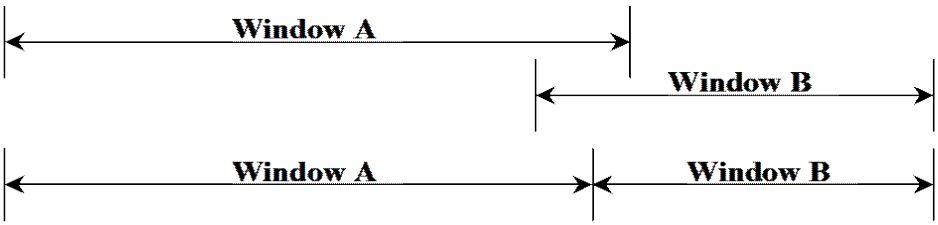
First, CompassCDS checks that the identification windows of the reference peaks do not overlap each other. If window overlap occurs, CompassCDS resolves the overlaps, and then the reference peak identification is processed.

Using the experimental reference retention times, CompassCDS calculates the other expected retention times, resolves the non-reference peak window overlaps, and the non-reference peaks are identified with these retention times and windows.

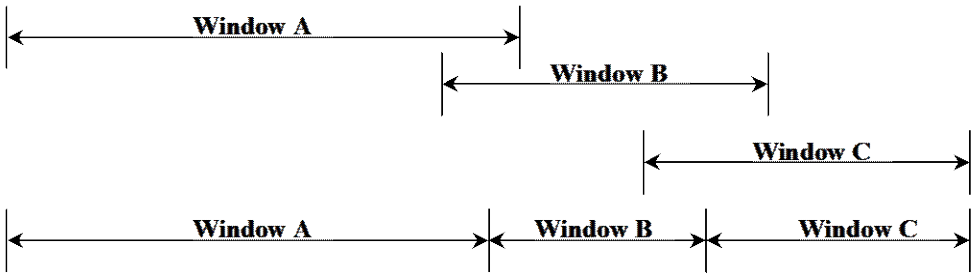
Since the reference and non-reference peaks are processed separately, it is possible to define larger reference windows because it does not matter if they overlap with the non-reference identification windows.

Resolving window overlap

If peaks are very close together, windows can overlap. This means that the end of an identification window can occur after the beginning of the next one. To cope with this problem, CompassCDS considers the common part of the windows, splits it in two, and assigns half to each window. For example:



If several successive windows overlap, the system resolves the first overlap (two first identification windows), then the next two ones. For example:



When using the relative identification windows (Window %), window overlaps can occur easily. If problems are encountered in peak identification, investigate what occurs during the window overlapping resolution.

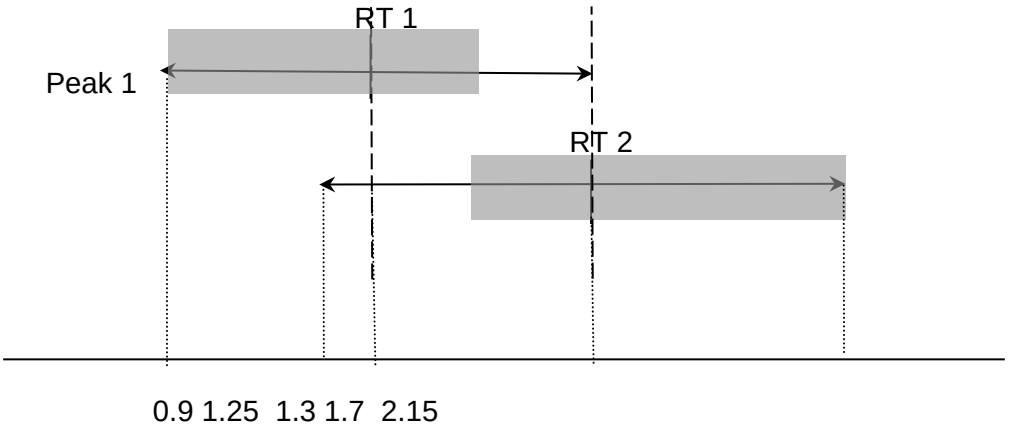
General Rule:

The window limit cannot go beyond the retention time of the previous or of the next peak. In this case the retention time of the previous/next peak is taken into account as the limit of the window, and the overlap is divided in two.

Example1: A peak retention time belongs to the identification window of another peak

Peak 1: RT1= 1.3 ID window: 0.4 min: [0.9 -1.7]

Peak 2: RT2= 1.7 ID window: 0.45 min [1.25 -2.15]



The identification window of Peak 1 becomes: [0.9-1.5] where 1.5 = RT1 + (RT2-RT1)/2

The identification window of Peak 2 becomes: [1.5-2.15] where 1.5 = RT2 - (RT2-RT1)/2

Example 2: a peak window belongs entirely to another.

Peak 1: RT1= 1.7 ID window: 0.45: [1.25 -2.15]

Peak 2: RT2= 1.99 ID window: 0.04 [1.95 -2.03]

The identification window of Peak 1 becomes: [1.25-1.97] where 1.97=RT1+ (RT2-RT1)/2

The identification window of Peak 2 becomes: [1.97 -2.03] where 1.97=RT2-(RT2-RT1)/2

Finding reference peaks

An identification window is defined for each peak.

A peak is identified as the reference peak if its retention time is found to be within the reference identification window. If there are no such peaks, the reference is not found.

If a reference identification window contains several peaks, the reference peak is chosen according to the selected reference window mode:

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the reference window.

Last: The peak will be the last peak found in the reference window.

Once the reference peaks are identified, CompassCDS will identify the other peaks.

Identification of the non reference peaks

Generally, the retention times are recalculated according to the two adjacent reference peaks. The formula for calculating the expected retention times for the non-reference peaks is:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_2 - RT_1}{RT_{ID2} - RT_{ID1}}$$

Where

RT is the expected retention time for a non reference peak.

RT1 is the real retention time of the reference peak preceding the peak.

RT2 is the real retention time of the reference peak following the peak.

RTID is the theoretical retention time of the peak defined in the identification table.

RTID1 is the theoretical retention time of the reference peak preceding the peak, defined in the identification table.

RTID2 is the theoretical retention time of the reference peak following the peak, defined in the identification table.

If peaks are eluted before the first reference peak: RT1 = RTID1 = 0. The index 2 is attributed to the next reference peak:

$$RT = RT_2 \frac{RT_{ID}}{RT_{ID2}}$$

If a peak appears after the last reference peak:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_1 - RT_0}{RT_{ID1} - RT_{ID0}}$$

Where RT0 and RT1 represent respectively the real retention times of the two reference peaks eluted before the peak of interest.

Note that this correction step works best when reference peaks are distributed throughout the entire chromatogram. In particular, be careful when using references that elute only at the beginning of a long run. They have a too strong impact on retention times at the end of the run. To minimize this effect, define a reference peak at the end of the run.

Once the system has calculated expected retention times for the remaining peaks, it centers the calculated identification windows on these times. If any windows overlap, the system will resolve the conflicts.

If several peaks fall within a window, the correct peak is chosen according to the selected identification mode:

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the identification window.

Last: The peak will be the last peak found in the identification window.

Note that if a reference peak is not found, its retention time will be the retention time set in the identification table, as if it had not shifted at all, therefore the identification of the peaks placed between the previous and the next reference peak may be affected.

If no reference peak is defined or found, peaks are identified by the retention times set in the identification table. Each peak retention time is compared to the identification window defined in the identification table.

Example:

For example, assume that three peaks exist in a chromatogram with theoretical retention times (saved in the identification table) of 5, 6, and 10 minutes.

When the sample is analyzed, the retention times have shifted to 6, 7.2, and 12 minutes. If the identification windows are 0.5 minutes wide, and reference peaks are not used, the peaks will not be identified.

However, if the last peak at 12 minutes is defined as the reference peak, and it elutes 1.2 times later than the defined theoretical retention time of 10 minutes, the expected retention times for the two other peaks (non-reference peaks) can be calculated.

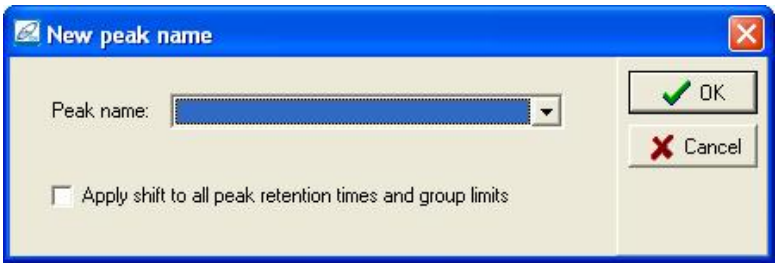
First peak: 5 x 1.2 = 6 minutes.

Second peak: 6 x 1.2 = 7.2 minutes.

The first two peaks can now be identified correctly with these new corrected retention times.

Peak re-identification

If a peak is bad identified by CompassCDS (due to a retention time shift for example), the user can re-identified it. Select the peak to re-identify in the chromatogram picture, then in the context menu, select the ‘Re-identification’ option. The following screen is displayed:



Select in the Peak name field, the name to assign to the selected peak. If you want that the software to apply the retention time shift to the rest of the peaks listed in the identification table, and to the group limits, select the ‘Apply shift to all peak retention times and group limits’ option. Note that the shift applied to the calculation of other peaks retention times or group limits is proportional to the time.

Group Identification

Result Groups and Calibration Groups

There are two types of groups: Result groups and Calibration groups.

- The result group adds the integration and quantification results of the compounds eluted in the time interval selected and /or the named peaks. The results are displayed in a table, displayed in the "results /group report" section of the chromatogram.
- The calibration group allows the user to quantify a group of peaks from a calibration curve or response factor. CompassCDS considers that all the integrated peaks present in the defined time period represent a single peak. A global calibration curve is built (or a global response factor entered in the calibration table) for the group. During this process, CompassCDS calculates a global quantity for the group (displayed in the group report), then sub-divides this quantity by peak according to its area percentage in the group and displays the individual results in the peak report: the ratio between peak quantity and the group quantity corresponds to the ratio between the peak area and the group area.

Do not forget to check the Cal. Box of each calibration group to be added in the calibration table. An interactive link exists between the peak and group identification tables and the calibration table.

The Group Identification Table

The group identification table contains four columns:

Group name	Group Type	Parameters	Cal.
GROUP1	Result group	0 range(s)	☐
GROUP2	Calibration group	0 range(s)	☐

Group Name: Specifies the name of the group.

Group type: Specifies whether the group is a result or a calibration group, which will induce the type of calculation that will be done for the group. It is possible to change it by accessing the list box.

Parameters: Defines the time limits (there can be several ranges) and/or names of the peaks to be added in the group.

Cal.: This column specifies the calibration groups to be quantified. A link exists between the group identification and the calibration table: each calibration group whose corresponding Cal. box checked is listed in the calibration table.

It is possible to either clear the entire table with the DELETE ALL popup menu (right click within the table) or delete single line as needed.

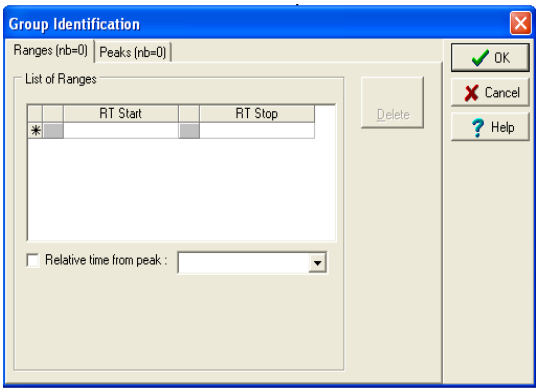
Identification of the Groups

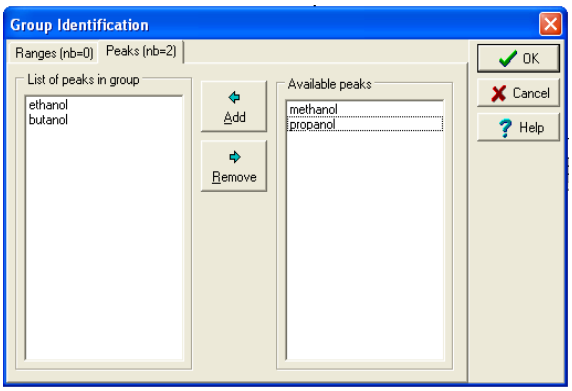
Peaks are added to a group based on their retention time or their name. It is possible to define a retention time interval or to select the name of the peaks to be added.

To add a group:

Click on Group identification in the browser.
Press the right mouse button in the group identification table.
In the popup menu, select ADD / RESULT GROUP or ADD / CALIBRATION GROUP.
Click in the Parameters column (left mouse button), and the Group identification dialog box appears.
In the Range page, enter the time limits of the intervals containing the peaks, or select them by dragging their name into the Peaks page.

- For the result group



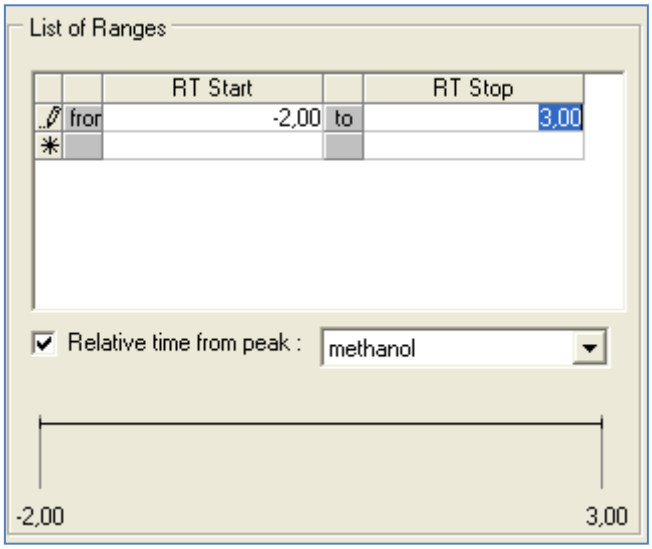


All results (area, height, quantity, etc.) of peaks belonging to the time range defined in the Range page and those named in the Peaks page are added.

NOTE: If 10 peaks are integrated within the time range of the group and only 3 are identified and quantified, then the group area will be the sum of the 10 peak areas. However, the group quantity will be the sum of the 3 peaks quantities (the quantity of the other 7 is considered to be equal to zero).

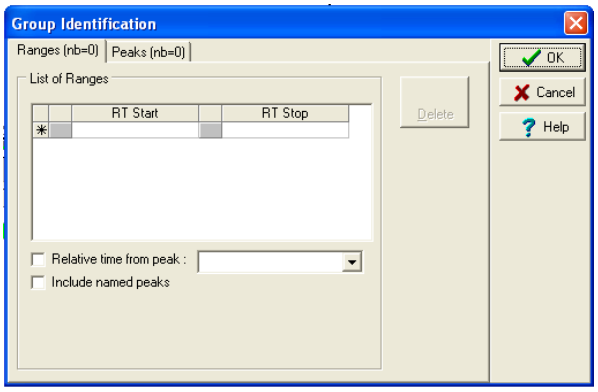
The time limits of a group can be defined relatively to a peak: In the Range screen, check the box ‘Relative time from peak’ and choose the name of a peak from the corresponding drop list: the

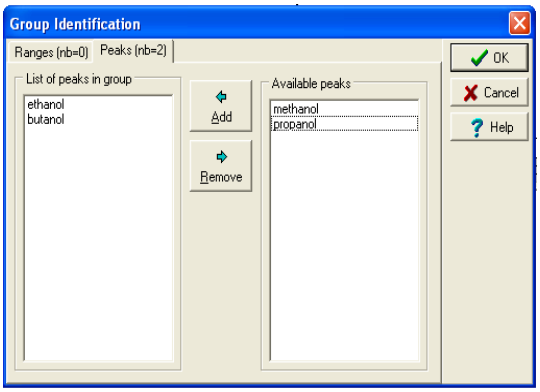
identification windows are defined based on the real retention time of this peak in the chromatogram. For example, to define a time range starting 2 minutes before the chosen peak and finishing 3 minutes after, define –2 and 3 in the time table and select the name of the peak in the ‘Relative time from peak’ scrolling list:



Several relative time intervals can be defined relatively to the same peak. To define those interval, select the peak name in the scrolling list and then define the interval times (take care to not overlay the intervals)

- For the calibration group:





By default the identified peaks whose retention times belong to the time range defining the group, are excluded from the group. To include them, select the option 'Include named peaks' or select their names in the page 'Peaks'.

The ‘Relative time from peak’ option has the same behavior than the one described in the result group section.

NOTE: In case a group is defined by a time interval: a peak is considered as a part of this group only if its apex belongs to the time interval defined. It is not necessary that both start time and stop time belong to the group time interval.

NOTE: In both cases, calibration group and result group, when reference peak(s) is (are) defined; the group interval time (based on a peak retention time) is calculated according to the recalculated peak retention time and not based on the theoretical one defined in the identification table. This allows correction of the shift of the retention times.

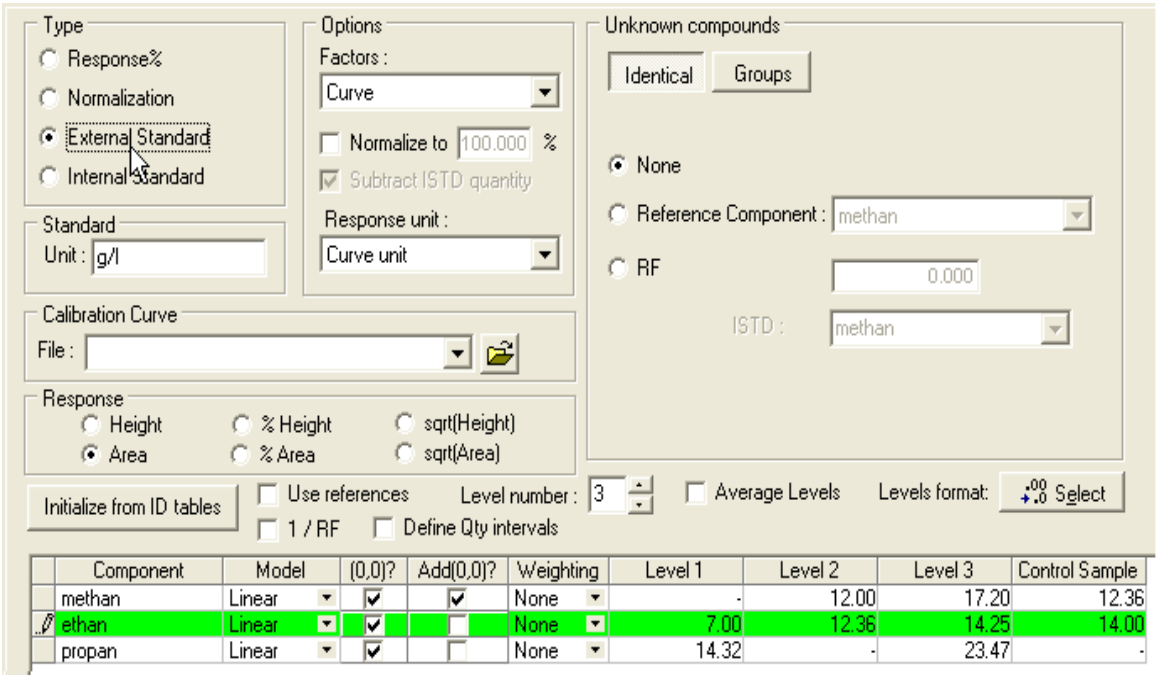
Quantification / Calibration

The aim of this step is to define the calibration parameters.

It is possible to work in two different calibration modes: Quantity versus Response or Response versus Quantity. The choice is made in the Configuration Manager.

Click on the calibration method in the browser to define the calibration parameters (or select the METHOD / PARAMETERS menu, or use the Ctrl+B key combination).

Now, define the different parameters for calibration: calibration type, response, factors, unknown compounds quantification, etc., proposed in the following screen.



Calibration Method Building

This part lists the steps to be followed in order to define a calibration method. Each step will be described in detail below.

In the Type section, select the calibration type. This selection determines how the quantification is calculated: Response %, Normalization, External Standard, or Internal standard. Details of these calibration types will be given in the paragraph "The Calibration Type" (see page 79).
To work with simple Response%, the calibration method is ready. For all other choices, additional parameters will need to be defined.
To work within the normalized mode (= external standard + normalization at a fixed percentage), check the Normalization option and enter the percentage value that the quantities will be normalized to in the 'Normalize to' field. By default, the results are normalized to 100 percent.
User can also check the External standard and the Normalize to cases, and enter the normalization percentage to obtain the same results.

It is also possible to normalize results in internal standard mode of calibration: check the 'Internal standard' and 'Normalize to' cases and enter the normalization percentage.
Define the response factor in the Factors field:

- Manual: If the response factor is known
- Curve: If the response factor is not known and that a calibration curve must be built
- Both: If some components have known response factors and others need the building of a calibration curve.

NOTE: If 'Curve' or 'Both' factor is selected, do not forget to enter a calibration curve name or select an existing calibration curve by pressing the button in the Calibration Curve section.

Specify the Response Unit in the corresponding field:

- Curve unit: Select Curve unit and precise this unit in the Standard Unit field (ppm, g/L, etc.)
- Mass%: To divide all the quantities by the sample mass (to display in the chromatogram properties) and multiply them by 100.
- Mass ratio: To divide all the quantities by the sample mass (to display in the chromatogram properties).

Note that in Normalization, only Curve unit is available.
In the Response section select the response mode. This selection determines how the peak will be processed- either by area, by height, by % area, % height, by area$^{1/2}$ or by height$^{1/2}$.
Configure the calibration table parameters:

- **Use references:** This option allows processing of one or several compounds listed in the table as another compound is defined in the table; which means with the same response factor or the same calibration curve. Enter in the 'Ref.' column the name of the reference peak.
- **1/RF:** This option allows user to enter inverse response factor.
- **Define Qty intervals:** This option allows user to define the interval in which CompassCDS must calculate the quantity of a compound, in the case of several solutions (polynomial models). Check the Use qty interval box for the concerned peaks, and enter the interval limits in 'Qty min' and 'Qty max' columns. If several solutions exist and this option is not selected, CompassCDS proposes the first strictly positive solution.
- **Level number:** to use for calibration building (curve or both factors). Enter the level number to use. The corresponding column number is displayed. The user has to complete those columns with the quantities associated to the level.
- **Average level:** When at least one calibration curve must be built, this option averages all the points of the same level before calculating the regression equation.
- **Levels format:** This option allows the user to modify the display format of the level entered in the table.

Calibration table filling: The content of the calibration table depends on the parameters selected: Calibration type, Response factor, Use reference, 1/RF, Define Qty intervals. The list of the columns that can be displayed is detailed underneath:

- **Component:** Lists the name of peaks and calibration groups to quantify in the table.

If the Cal. is checked for peaks and calibration groups in the peak and group identification parts in the method, they are automatically listed.

If all peaks and calibration groups (defined in the identification tables) must be listed in the calibration table, click onto the Initialize from ID tables' button. All the Cal cases will be automatically checked in the identification tables. An interactive link exists between identification tables and calibration table.

Note that peaks are listed in chronological order. Calibration groups are listed after the peaks, by definition order.

- **ISTD?** This column is displayed if the Internal Standard calibration type is selected. It allows entry of those components which are internal standards.
- **ISTD Name:** This column is displayed if the Internal Standard calibration type is selected. It allows association of an internal standard to each peak or calibration group.
- **Ref:** This column is displayed if the Use references option is selected. It allows definition of the peaks that will be used as reference for the quantification of other ones.
- **Model:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows the user to choose the mathematical model used for the calibration curve building
- **(0;0):** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'curve' or 'both'. It allows the user to force the curve pass through the point (0,0).
- **Add(0,0)?:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows the user to use the point (0,0) as a calibration point for the curve building. The curve will not necessarily pass through the origin, but the origin is taken into account for the calibration curve equation calculation.
- **Weighting:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows entry of a weighting of points during the calibration curve building.
- **Level-I:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is curve or both. It allows entry of the quantity of the compound for the calibration level I. If the compound is missing from the standard sample, enter '-' in the calibration table. No point will be added in the corresponding calibration curve for that level.

Response factor or 1/RF: This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'manual' or 'both'. It allows entry of the response factor for the compound or its inverse if the 1/RF option is selected.

- **Manual factor:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'both'. It allows entry of the components that will have a response factor.
- **Use Qty interval:** This column is displayed if the Define Qty intervals option is selected. It allows entry of the quantity calculation interval. This is useful when polynomial model is used, because several solutions can exist.
- **Qty min:** This column is displayed if the Define Qty intervals option is selected. It allows entry of the lower limit of the interval.
- **Qty max:** This column is displayed if the Define Qty intervals option is selected. It allows entry of upper limit of the interval.

This sets the way the unknown compounds (integrated peaks but not identified) are quantified. Two options are proposed: quantify all unknown compounds similarly by selecting the identical tab or according to retention time intervals by selecting the Groups tab.

Identical process for all unknown peaks:

- Choose none in the ‘Unknown compounds’ field to not quantify unknown peaks. The quantity of unknown peaks displayed in the result table is equal to 0.
- Choose Reference component to quantify unknown compounds by the same way as a peak present in the calibration table, and select the name of this peak in the scrolling list. If the calibration type is ‘Internal standard’, the internal standard associated is the one associated to the selected peak.
- Choose Response factor to quantify unknown compounds according to a response factor (RF or 1/RF whether the option 1/RF is selected or not) and enter the value of the response factor in the corresponding box. If the calibration type is ‘Internal standard’, select the name of the associated internal standard.

Unknown peaks are processed according to their retention time:

- Define the interval number in the ‘Groups’ tab, by activating the + and – buttons, and enter the start and the end of each group in minutes. Then enter for each group the way the peaks will be quantified (see previous paragraph).

The Response Mode

First, choose the response mode, to indicate whether the quantities are a function of the area, the height, the area %, the height %, area$^{1/2}$ or height$^{1/2}$ of the peaks.

By default, quantities are a function of the peak areas.

The Calibration Type

There are four options for calibration: response percentages, external standard, internal standard, and normalization. (The normalization type corresponds to normalization in external standard.)

Response Percentage

This is the simplest calibration mode, which is calculated based on the assumption that all integrated peaks have a response factor of 1, and therefore, the quantity associated with each peak corresponds to the ratio of its response (area, height, area%, height %, area$^{1/2}$ or height$^{1/2}$) over the sum of the response of all peaks.

The quantity Q of a compound is

$$Q = \frac{R}{\sum R} \times 100$$

Where

R is the response (area, height, area%, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

$\sum R$ is the sum of the responses of the chromatogram peaks

NOTE: When the results are normalized, the divisor and the multiplier factors cannot be used to modify the quantities.

NOTE: In response percentage mode, the results are always expressed in area% independently of the response mode: area, area%, area$^{1/2}$ (also, for height, height% or height$^{1/2}$, the results are always expressed in height %).

External Standard

Three response factor types are available: Manual, allowing user to manually enter the response factor of every peak to be quantified; Curve, allowing the building of calibration curves for all peaks; both, allowing the use of both curve and manual factors within the same method.

Manual Response Factors:

Choose ‘manual’ in the factors box.

In the case of manual response factors, the quantity Q of a compound is

$$Q = RF \times R \times \frac{M}{D}$$

Where

RF is the response factor of the compound read from the calibration table.

R is the response (area, height, area % height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

D is the divisor factor.

M is the multiplier factor.

Select ‘Curve unit’ in the response unit list box in order not to express the results in mass ratio or percentage, but in the same defined unit.

When the quantities are calculated, they can be manipulated as follows:

- They can be expressed in mass ratio relating to the sample mass:

The quantity Q of a compound becomes

$$Q = \frac{RF \times R}{m} \times \frac{M}{D}$$

where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

m is the mass of the sample (entered prior to acquisition, editable and modifiable in the chromatogram properties).

D is the divisor factor.

M is the multiplier factor.

To express the results in mass ratio, select Mass ratio in the Response unit list box.

- They can be expressed in Mass percentage relating to the sample mass:

The quantity Q of a compound becomes

$$Q = RF \times R \times \frac{100}{m} \times \frac{M}{D}$$

Where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

m is the mass of the sample (entered prior to acquisition and can be edited or modified in the chromatogram properties).

D is the divisor factor.

M is the multiplier.

To express the results in mass percentage, select 'Mass %' in the Response unit list box.

- They can be normalized to any strictly positive real number, up to 100. If this real number is Norm:

The quantity Q of a compound is

$$Q = \frac{RF \times R}{\sum (RF \times R)} \times Norm$$

Where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

Norm is the value of percentages normalization.

NOTE: As the results are normalized up to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

To obtain normalized results, check the Normalization box and enter the expected percentage.

NOTE: An alternative processing method is to choose the Normalization response type and then define the normalization percentage in the corresponding box.

NOTE: If the 1/RF option has been selected, the user enters the value of the inverse response factor in the calibration table and CompassCDS will calculate the value of the corresponding RF in order to apply the same calculations.

Curve Factors

Choose Curve in the 'Factors' box.

In case factors are read from a curve (Factors=curve), the calibration curve must first be built.

Calibration curve building:

When a calibration point is added to the curve, its coordinates are the response of the compound and the associated quantity.

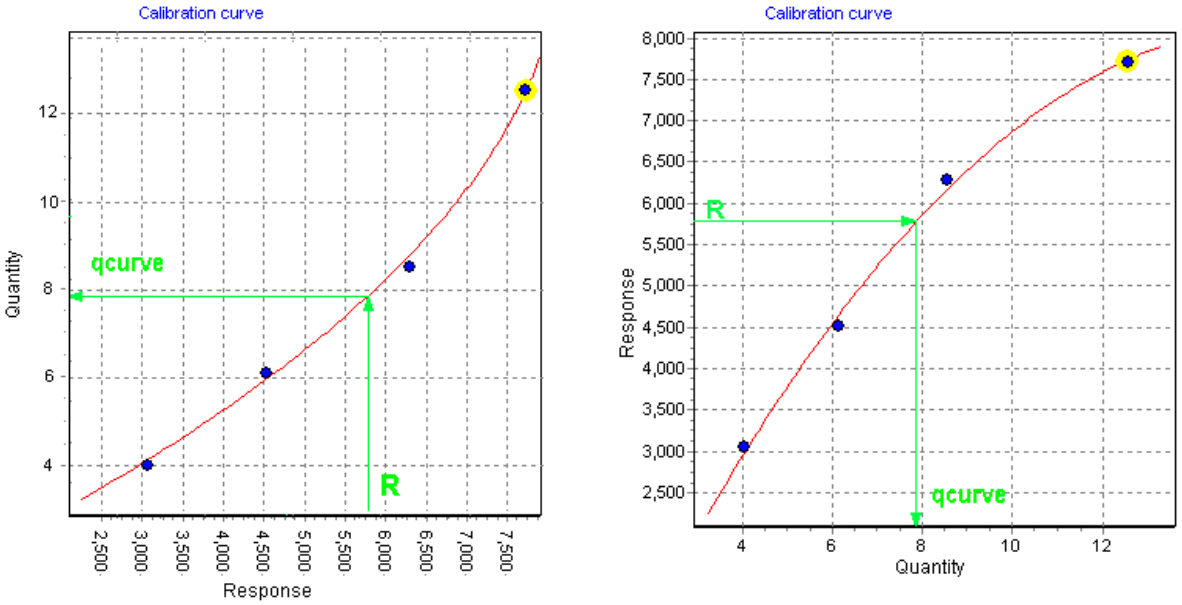
$q_{curve} = Q$ entered in the calibration table

NOTE: The multiplier and the divisor factor are not taken into account for the calibration curve building, except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

NOTE: If the response unit is 'Mass ratio' or 'Mass %', do not forget to enter a sample mass in the chromatogram properties, otherwise CompassCDS will not be able to build the calibration curve (even if the mass is not taken into account for the calibration curve building).

Quantification of unknown samples

The quantification of unknown samples is made using the calibration curve: a response corresponds to a quantity.



Quantity versus response orResponse versus quantity

The quantities read from the calibration curves are then corrected with M and D factors and turned into mass ratio or mass percentages:

If the Response unit is **Curve unit:**

$$Q = q_{curve} \times \frac{M}{D}$$

If the Response unit is **Mass ratio:**

$$Q = \frac{q_{curve}}{m} \times \frac{M}{D}$$

If the Response unit is **Mass percentage:**

$$Q = \frac{q_{curve}}{m} \times \frac{M}{D} \times 100$$

Results can also be **normalized:**

The quantity QNorm of a compound is:

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where Q is the quantity of the peak calculated in curve unit

$\sum Q$ is the sum of the quantities of the peaks

Both Factors

It is possible to work both with manual factors and calibration curves for the same chromatogram: Choose Both in the Factor zone. In the calibration table, the boxes in the column “Manual” must be checked for the compound whose factor is entered manually, then enter the manual factors in the corresponding column. For the other compounds, fill all the Level columns.

Note that the multiplier and the divisor factor are not taken into account for the standard calculation (Calibration curves building), except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

Internal Standard

The purpose of the internal standards is to compensate for the amount of injected sample when it can vary. If there are several internal standards, it is necessary to choose which internal standard is associated to each of the compounds.

As for external calibration mode, it is possible to use manual response factors, curve factors or both. Whichever process is selected, the user must still enter the quantity of the internal standard(s) for each chromatogram. These quantities can be entered:

- In the acquisition window for a Quick Start.
- In the 'Istd values' column for a sequence or a reprocessing list.
- In the chromatogram properties for a single reprocessing.

NOTES: When working in a curve factor unit, do not enter the internal standard quantity (ies) in the corresponding line of the calibration table; these values will be ignored.

In order to reprocess a chromatogram where the quantification method is different from internal standard (% response or external standard), using the reprocessing single functions (see page173), 2 steps must be performed:

First, reprocess the chromatogram as an unknown with the internal standard calibration method (in the 'method file' box). This step allows the user to define which compound(s) is/are internal standard(s).

Second, reprocess a second time the sample as an unknown or standard and enter the quantity of the internal standard(s) in the chromatogram properties.

Manual Response Factors:

Choose manual in the Factors box.

The response factors to enter are ‘Relative factors’, which means the response factor of the peak divided by the response factor of the associated internal standard. The response factor of the internal standard must thus be equal to 1.

In case of manual response factors, the quantity Q of a compound is

$$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Where

Qistd is the quantity of the associated internal standard, entered by user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier factor.

Select Curve unit in the response unit list box to express the results in user unit (g/L, ppm, etc.)

- Quantities can be expressed in mass ratio, relating to the sample mass:

The quantity Q of a compound becomes

$$Q = \frac{Q_{istd}}{m} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Where:

Qistd is the quantity of the associated internal standard, entered by the user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier factor.

m is the mass of the total sample including the internal standard mass(es) (entered prior to acquisition editable and modifiable in the chromatogram properties).

To express the results in mass ratio, select Mass ratio in the Response unit list box.

- Quantities can be expressed in mass percentage, relating to the sample mass:

The quantity Q of a compound becomes

$$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{100}{m} \times \frac{M}{D}$$

Where

Qistd is the quantity of the associated internal standard, entered by the user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier.

m is the mass of the total sample including the internal standard mass(es) (entered prior to acquisition editable and modifiable in the chromatogram properties).

To express the results in mass percentage, select ‘Mass %’ in Response unit list box.

- Quantities can be normalized to any strictly positive real number, up to 100. If this real number is Norm:

$$Q' = \frac{Q}{\sum Q} \times Norm$$ Where $$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Q is the quantity of the compound before normalization, and ΣQ is the sum of the quantities of the compounds before normalization. If the box Subtract istd mass is checked, the quantities of the internal standard(s) will be zero and will not be taken into account in ΣQ.

Note that as the results are normalized up to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

NOTE: If the option 1/RF has been selected, the user enters the value of the inverse response factor in the calibration table, CompassCDS calculates the value of the corresponding RF, and then applies the same calculations.

Curve factor

The relative response factors (response factor of the peak divided by the internal response factor) can be calculated from a calibration curve. For a compound or a calibration group, the quantity corresponding to the response is read from the calibration curve. This means that a calibration curve must first be built.

Calibration curve building

When a calibration point is added to a curve, its coordinates are the relative response of the compound and the relative associated quantity. The response is the response of the compound divided by the response of the internal standard. The relative quantity is the quantity entered for the compound in the calibration table divided by the internal standard quantity.

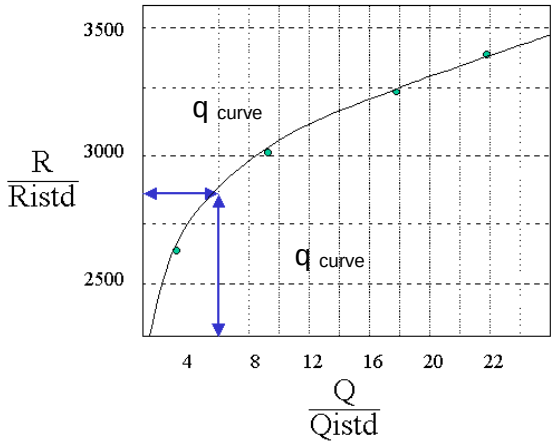
$$q_{curve} = \frac{Q}{Q_{istd}}$$

Q is the quantity of standard entered in the calibration table.

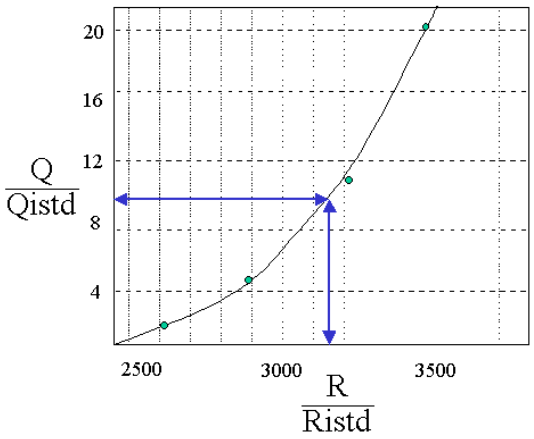
Qistd is the quantity of the internal standard entered in the acquisition window (Quick Start or sequence). Qistd can be modified in the chromatogram properties.

Note that the multiplier and divisor factors are not taken into account for the calibration curve building , except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

Quantification of unknown samples



Response versus quantity



Quantity versus response

For unknown samples, the calculation is the same as for the manual factor mode, except that the quantity ratios are read from the curve.

Those quantities are then corrected with the factors M and D and can be expressed as mass ratio or mass percentages:

If the Response unit is Curve unit:

$$Q = q_{curve} \times Q_{istd} \times \frac{M}{D}$$

If the Response unit is **Mass ratio:**

$$Q = \frac{q_{curve} \times Q_{istd}}{m} \times \frac{M}{D}$$

If the Response unit is **Mass percentage:**

$$Q = \frac{q_{curve} \times Q_{istd}}{m} \times \frac{M}{D} \times 100$$

Results can also be **normalized:**

The quantity QNorm of a compound is:

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where

$\sum Q$ Is the sum of the quantities of the peaks

For both mass ratio and mass% unit, m is the mass of the total sample including the internal standard mass (es) (entered before acquisition, editable and modifiable in the chromatogram properties).

Both Factors

It is possible to work with both manual factors and calibration curves for the same chromatogram: Choose Both in the Factor zone. The boxes in the column Manual must then be checked for the compound whose factor is entered manually in the calibration table.

Note that the multiplier and the divisor factor are not taken into account for the standard calculation (calibration curves building), except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

GENERAL NOTE FOR INTERNAL STANDARD CALIBRATION: It is possible to express the results after removing the internal standard quantities by checking the subtract ISTD mass option. This option is available with the three response unit proposed: curve unit, mass ratio and mass%. In the case of the response in curve units, the quantity of internal standards in the result table is equal to 0, and not included in the total quantity displayed.

In the case of the response in mass ratio or mass %, the quantity of the internal standard displayed in the result table is equal to 0, and for the calculation of the quantity of the other peaks, the mass taken into account is the mass entered by the user minus the sum of the quantities of the internal standard compounds.

The mass to enter is the sample mass after the addition of internal standard(s).

In the case of normalization, if Subtract ISTD mass is checked, the quantity of internal standard(s) is 0, and is not included in ΣQ.

Normalization

The normalization mode allows the user to calculate the ratio between each peak quantity, quantified using external calibration and the sum of all peak quantities, quantified using the same mode.

Note that the result is the same as the one obtained when selecting External calibration, checking normalization and defining a percentage in

.

The quantity QNorm of a compound is

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where

Q is the quantity of the peak (calculated as described in the previous sections of the manual, according to the response mode: curve unit or manual factors)

$\sum Q$ Is the sum of the quantities of the chromatogram peaks

Norm is the value to which the percentages are normalized. By default, they are normalized to 100. Note that as the results are normalized to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

Response Factor Calculation: RF

The response factor is a variable calculated automatically by CompassCDS, equal to the quantity divided by the response. A response factor is calculated for each quantified peak or group, whatever the mathematical model defined in the case of 'Curve' factor.

The response factor of an unknown sample does not take into account:

- Multiplier factor
- Divisor factor
- Normalization factor
- Sample mass

CompassCDS proposes two variables 'RF' and 'recomputed RF', calculated as described in the following table:

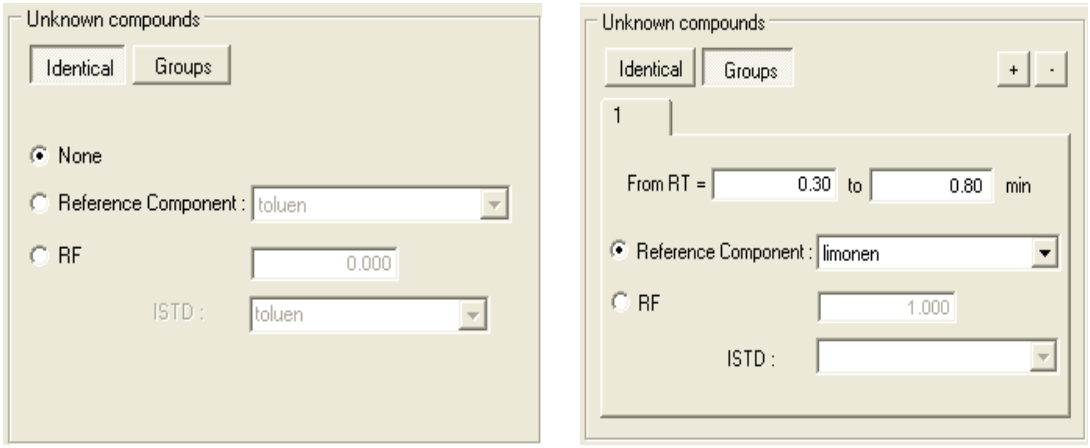
	CURVE factor		MANUAL factor	
Sample Type	RF	RF_Rec	RF	RF_Rec
Standard	$\frac{\text{Qty table}}{\text{Response}}$	$\frac{\text{Qty curve}}{\text{Response}}$	RF table	$\frac{\text{Qty}}{\text{Response}}$
Unknown	$\frac{\text{Qty curve}}{\text{Response}}$	$\frac{\text{Qty curve}}{\text{Response}}$	RF table	$\frac{\text{Qty}}{\text{Response}}$

Where Qty table is the quantity entered by the user in the calibration table, Qty curve is the quantity given by the calibration curve, and Qty is the quantity calculated by CompassCDS without taking into account the multiplier and divisor factors, the normalization factor and the sample mass.

In the case of internal standard, the calculated response factor is the relative response factor. It is equal to the ratio of the compound RF divided by the RF of its internal standard. The response factor of the internal standard is thus equal to 1.

A variable named RRF (reverse response factor 1/RF) can also be displayed in the result table.

Unknown Peak Processing



Unknown peaks (integrated but not identified) can be either all processed in the same way by using 'Identical' tab, or processed by groups defined according to time periods by using the 'Groups' tab.

Identical process for all unknown peaks:

It is possible to process unknown compounds in three different ways:

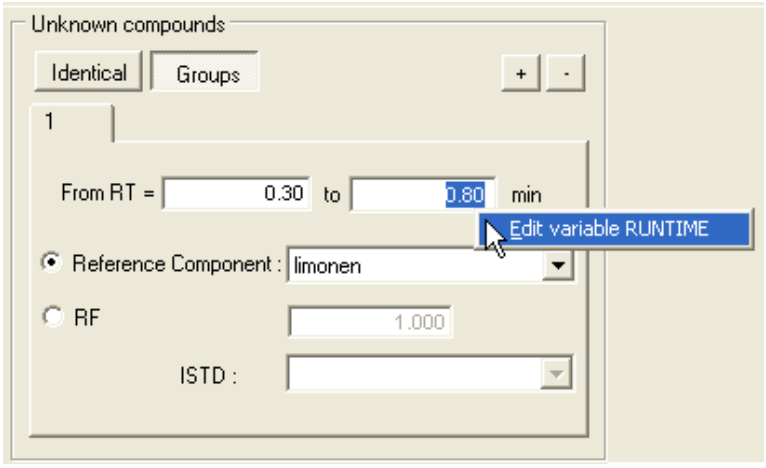
- **No processing:** Choose none in order not to quantify unknown compounds. A response factor of zero will be assigned for all unknown peaks.
- **Reference component:** In this case, the unknown samples will have the same response factor as the one specified in the list box. The reference peak is listed in the calibration table.
- **Response factor:** In this case, the unknown samples will have the response factor specified in the edit box, by default, this factor is one.

NOTE: If the calibration mode is internal standard, and if unknown peaks are processed with a response factor, it is necessary to choose the internal standard associated with unknown peak(s) in the internal standard box. Only one choice is available for all the unknown peaks.

Unknown peaks process according to retention time (groups):

It is possible to divide the chromatogram into time periods, and to process each period (group) differently. The group number is defined by activating + and – buttons. For each group, define the time period, and then choose the process to apply. The options proposed are the same as the 'Identical' tab ones.

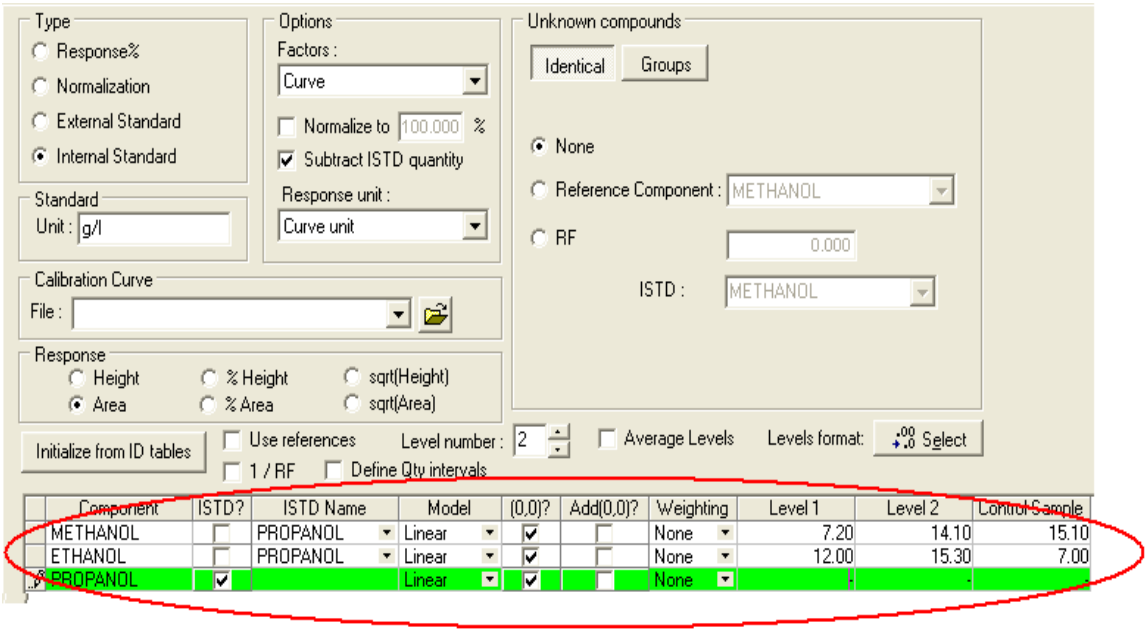
NOTE: It is possible to configure the format (number of significant digits, scientific format) of the group time limits and of the RF variable. Put the mouse cursor on the variable box that is to have its format changed, click on the right mouse button and select the 'Edit Variable XXX' option in the popup menu (XXX represents the variable name).



The variable screen is displayed and only allows the modification of the format for the selected variable.

The Calibration Table: As a Preliminary Step to a Calibration Curve Building

In the cases where the Curve and Both factors have been selected, the calibration table has to be completed.



If the user has checked the Cal. Boxes for peaks and calibration groups in the identification table, the names of these peaks and groups to be quantified are automatically imported into the calibration table. If a user wants all of the defined peaks and calibration groups to be imported into the

calibration table, without checking all the corresponding ‘Cal’ boxes, he must click on the ‘Initialize from ID table’s’ button.

A Control Sample column is displayed in the table. It allows the user to realize a suitability test on a control sample, by comparing the experimental quantity of the peak (in the control sample chromatogram) to the value defined in the table. Note that this value is theoretical and does not correspond to a calibration point.

Peaks are listed according to their retention time; calibration groups are displayed at the end of the list in their creation order.

A name must be defined in the Calibration Curve box, which is the name of the calibration file. This file will contain the curves for all the compounds defined in this table.

The number of calibration levels must be specified in the ‘Level number’ box, the corresponding column number will be displayed. The user must complete the table.

- **Model:** Several mathematical regression models are available:

Point to point: The calibration curve is composed of lines drawn between the calibration points.

Polynomial: It is possible to modify the order of the polynomial. A calibration curve can be modeled with up to a 5th order polynomial. The regression polynomial can be forced through zero (for example, in the case of a one-point calibration, the polynomial will be of order one and forced through zero).

If there are not enough points for calculation (e.g. only one point available for a 2nd order polynomial), the order of the polynomial is reduced and a message is displayed in the panel (below the polynomial coefficients).

Power: This is a $y= ax^b$ model.

Exponential: This is a $y=ae^{bx}$ model.

Logarithm: This is a $y=a + b \ln x$ model.

Average RF: Environmental laboratories in the USA routinely use a number of EPA approved methods and report formats for GC and GC/MS determination of analytes in matrices such as soil, air or water. Many of these methods require the use of the average response factor. To fit that need, CompassCDS provides a special model called Average RF.

If that model is chosen, it will imply automatically a linear model, force (0, 0) and 1/x2 weighting for the curve building. When the Averaged RF model is chosen, the other options which are set automatically cannot be changed until the calibration mode is changed.

- **(0; 0)?** Force the curve to go through (0;0).
- **Add (0, 0)?** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is curve or both. It allows the user to use the point (0,0) as a calibration point for the curve building. The curve will not necessarily pass through the origin, but the origin is taken into account for the calibration curve equation calculation.
- **Weighting:** Different weighting models are available:

None: Gives the same importance to all calibration points.

x: This model calculates each calibration point using a weight proportional to the abscissa of the curve.

x^2: This model calculates each calibration point using a weight proportional to the square of the abscissa.

1/x: This model calculates each calibration point using a weight proportional to the inverse of the abscissa.

$1/x^2$: This model calculates each calibration point using a weight proportional to the square of the abscissa inverse.

log x: This model calculates each calibration point using a weight proportional to the decimal logarithm of the abscissa.

ln x: This model calculates each calibration using a weight proportional to the natural logarithm of the abscissa.

1-N: In this model, the weight of each new point is equal to the sum of previous point weights. For example, for 5 points, the weights are respectively: 1, 1, 2, 4, and 8.

- **Level-I:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is curve or both. It allows entry of the quantity of the compound for the calibration level-I. If the compound is missing from the standard sample, enter '- 'in the calibration table. No point will be added in the corresponding calibration curve for that level.
- **Average levels:** If this option is checked, CompassCDS will average all calibration points of the same level (by compound) before building the calibration curve.
- **1/RF:** If this case is checked, the user has to enter the inverse of the RF (if manual response factor mode is used) in the corresponding column of the calibration table, and in the unknown compounds process field, if the unknowns are processed with manual response factor.
- **Use references:** A column 'Ref' appears. This option allows one or several compounds listed in the table to use the same calibration as another compound defined in the table that means with the same response factor or the same calibration curve. Enter in the 'Ref.' Column the name of the reference peak.
- **Define Qty intervals:** Three more columns are displayed, 'Use qty interval', 'Qty min' and 'Qty max'. This option allows user to define the interval in which CompassCDS must calculate the quantity of a compound, in the case of several solutions (polynomial models). Check the 'Use qty interval' box for the concerned peaks, and enter the interval limits in 'Qty min' and 'Qty max' columns. If several solutions exist and this option is not selected, CompassCDS uses the first strictly positive solution.

A Few Examples for Calibration

If you are not sure of how to configure the calibration method, please review the following examples which may be helpful.

1. External Standard with Calibration Curve building

To perform an external calibration, create a calibration curve for each compound of interest using standard samples. The amounts of each analyte in the standard samples for each level must be entered in the calibration table. These calibration curves are then used to determine the amount of each analyte in unknown samples.

The results for unknown samples are expressed in the same unit as the calibration samples.

How to proceed

- First, define the peak identification table.
- Then, in the calibration method: Choose External standard as the calibration type.
- Choose the response (Area, Height, Area %, Height %, and area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose Curve (since response factors are not yet known).
- In the calibration curve area, define the name of the curve to be built (or choose an already existing curve name using the open file box).
- Press the Initialize from ID table's button to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatically.
- Above the calibration table, enter the number of calibration levels to be used and then specify the quantities of the compounds for each level in the calibration table. Each calibration level corresponds to a calibration standard.

The calibration method is ready.

Calculation of relative response factor

To specify response factors relative to a reference compound, a user must create variables. Two cases are treated according to the reference compound remains the same or not.

How to proceed

Fixed reference compound: For example, if this reference compound name is 'Benzene', a variable called 'Relative RF' must be created, which would be a peak variable with the following formula: 'RF/RF('Benzene')', then the relative response factors can be displayed in the peak result table.

Variable reference compound: Two variables must be created. The first one could be called 'Ref Name', which would be a global and user input variable. The second one could be called 'Relative RF', which would be a peak variable with the following formula: 'RF/RF(Ref Name)'. A default value (name of the reference compound) can be specified in the acquisition method and the reference compound can be changed before each run in the acquisition window. The relative response factors can then be displayed in the peak result table.

Normalization to a Value

The sum of the compounds present in the sample to analyze represents a well-known percentage of the mother solution (50% for example). The response factors of peaks to quantify are known.

The results should be expressed in quantity percentages.

How to proceed

- First, specify the peak identification table.
- Then in the calibration method: Choose Normalization as the calibration type.
- Choose the response (Area, Height, Area %, Height %, area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose 'Manual'.
- In the next edit box (Normalize to) enter the value to which the results should be normalized: 50.
- Press the 'Initialize from peak ID table' button to import all the identified peaks, or check the 'Cal'. Box of each peak of interest in the identification table to make the import automatically.
- In the calibration table, specify the response factors for each of the peaks and calibration groups.

The calibration method is ready.

NOTE: If you want to quantify unknown compounds and give them a response factor of 1, select in the ‘unknown compounds zone response factor’ and enter 1.

Internal Standard, Result in Mass %.

Build a method to analyze sample owning defined peaks and groups in internal standard calibration type. The user knows the relative RF of each peak and calibration group. Unknown peaks are processed with the RF of an identified peak.

The results should be expressed in percentages of total sample weight.

How to proceed

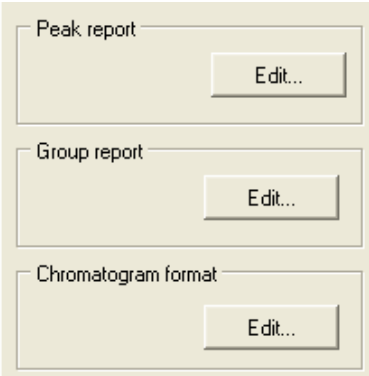
- First, specify the peak and group identification tables, take care to specify Calibration groups for the groups containing only the peaks that must be quantified with the same response factor.
- In the calibration method: Choose Internal standard as the calibration type.
- Choose the response (Area, Height, Area %, Height %, and area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose Manual.
- In the Response unit zone, choose Mass % (since the responses are to be divided by sample mass and multiplied by 100).
- In the Unknown compounds zone, select the identical tab, check ‘Reference component’ and choose the name of the reference component.
- Press the ‘Initialize from ID table’ button to import all the identified peaks, or check the ‘Cal.’ box of each peak of interest in the identification table to make the import automatically.
- In the calibration table, specify the internal standard and the response factors of each peak and calibration group.

The calibration method is ready.

If the internal standard quantity is strictly the same for standards and unknowns, you should enter this quantity in the method acquisition part before chromatogram acquisition. It will be possible to modify this value in the Quick Start window or in the sequence.

Formats

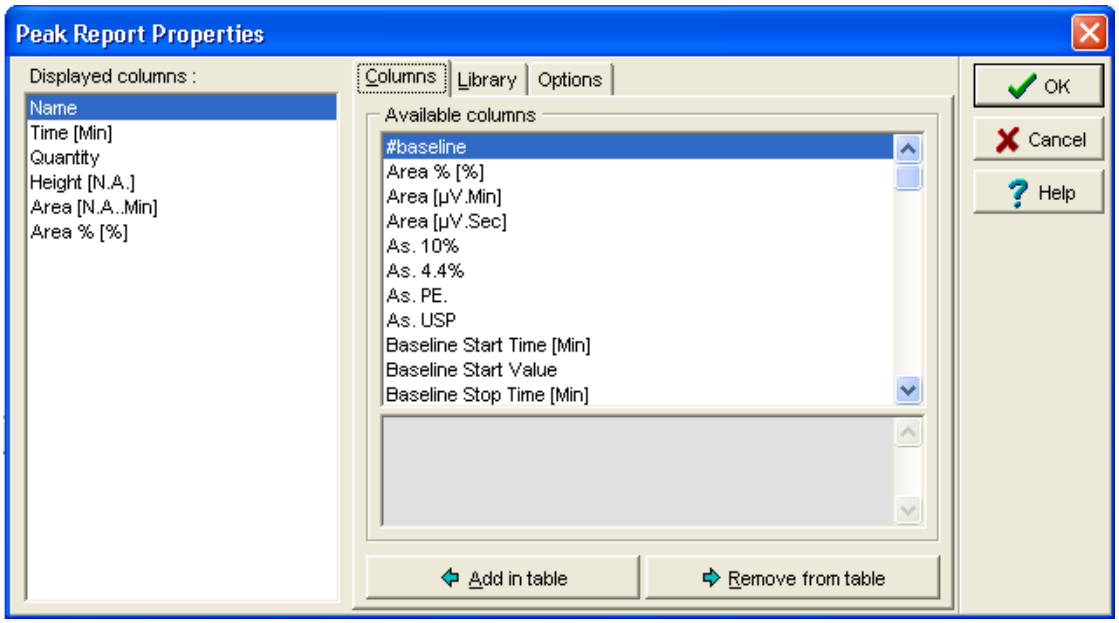
This section is accessible from the method or using the shortcut Ctrl+F, allows configuration of chromatogram, peak table and groups table formats.



The Peak Table Format

The purpose of the option is to configure the columns to display in the peak results table. Click on the Edit button in the ‘Peak report’ part.

The following screen is displayed:



NOTE: This screen is also accessible from the result peak table. Click on the right mouse button in the table, and choose REPORT PROPERTIES in the popup menu. The peak report properties appear.

This screen is composed of three sections:

Displayed columns: In this section, the variables to be displayed in the result table are listed in the right order.

Available columns: In this section, the variables calculated by CompassCDS are displayed. In order to make the software calculate another variable, define the variable in the variable editor (peak variable), and then it will appear in the available columns.

The gray section placed under the ‘Available column’ zone displays a description of the variable selected in the ‘Available column’ zone.

To add or remove a column from the report: Either click and drag the variables from the ‘Available column’ zone to the ‘Displayed column’ zone or from the ‘Displayed column’ zone to the ‘Available columns’ zone or select them with the mouse and click on the buttons

and

, or double-click on the name of the variable to add in the 'Available columns' or on the name of the variable to remove from the table in the 'Displayed columns'.

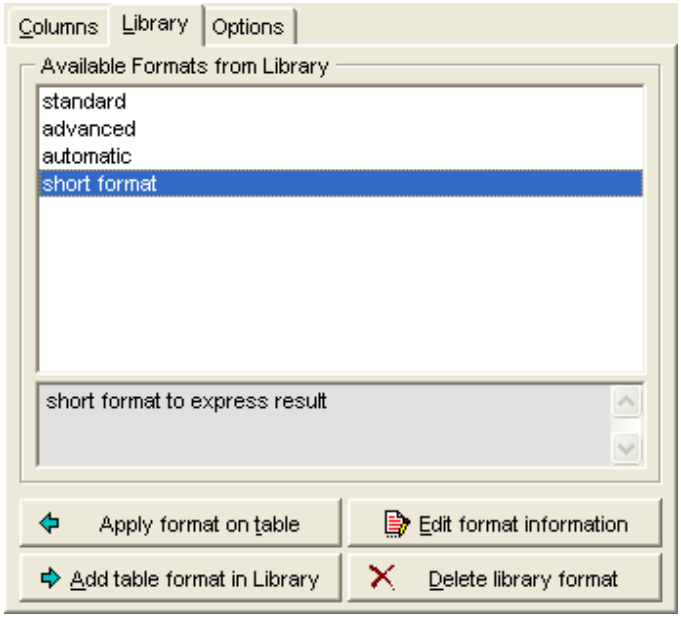
To change the report column order: In the ‘Displayed column’ zone, click and drag the variable to modify their order in the table:

The options page:

- **Show unknown peaks:** By default unknown peaks are shown in the peak table. But when this box is unchecked, only the identified peaks are displayed. When no peak is displayed in the peak report, it indicates that no peak is identified and this box is checked.
- **Display index column:** A column corresponding to the peak indices is displayed in the peak report. It is possible to hide this column by unchecking this box.
- **Show missing peaks:** The missing peaks (not identified in the chromatogram) are listed in the result table with their theoretical RT. The ND (not defined) value is assigned to other variables.

The Library page

It can be of interest to save a format as template, to apply it in several method, or printed report, or expected files. To do that, select the library tab, the following screen is displayed:



Click on the

button. A window appears, in which the name of the format can be saved with an entry field to provide a short description of the format.

The format is then added to the available formats. By clicking on the format, the description of the format is displayed in the gray zone.

In a different method, click on Apply format on table, and the peak report format is displayed in the 'Displayed column' zone.

To delete an obsolete format, select the format and click on Delete library format.

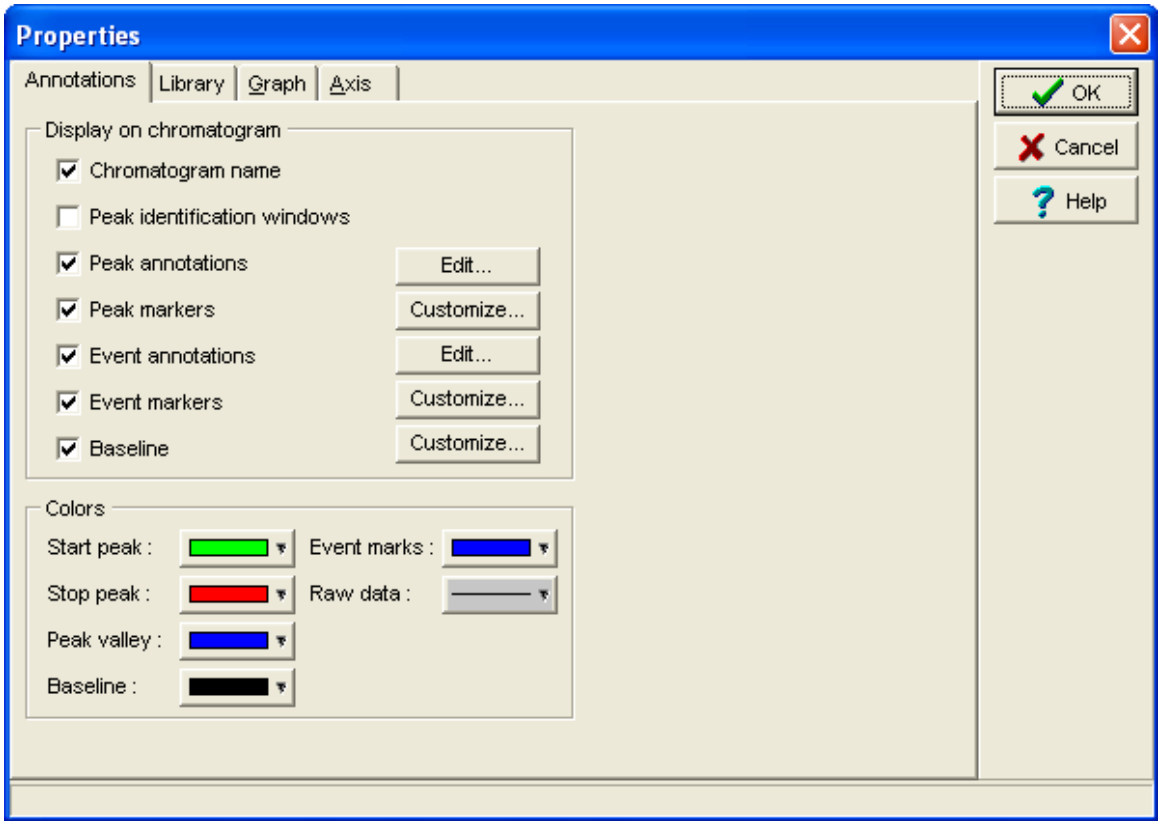
To change the name or the description of a format, select the format and click on Edit format information.

The Group Table Format

The group table can be customized as the peak table, e.g., in the report properties it is possible to change the displayed variables and to create formats. These formats will be accessible from CompassCDS Report Editor and in other methods or chromatograms. It is also possible to save group formats in a library.

The Chromatogram Format

Click on the Edit button in the "Chromatogram format". The following screen is displayed:



Four tabs are proposed: Annotations, Library, Graph, and Axis.

Annotations

- Check or Uncheck Chromatogram name to display or not the name of the chromatogram onto the chromatogram chart. This can be useful to copy/paste the chromatogram picture from CompassCDS to another application (Word, Paint, etc.) without the chromatogram name. This option is also applied when printing a chromatogram from the Workspace option (see corresponding chapter).

NOTE: If saving a library without the ‘Chromatogram name’ option, and use this format in the report style/ Chromatogram object, the name of the chromatogram will nevertheless be printed on the chromatogram picture.

- Check Peak identification windows to display the identification windows on-screen (Corresponds to pressing the icon). The peak identification windows are shown only one after the other when the identification method is displayed: The identification window will be displayed when the corresponding line is selected in the peak identification table.
- Check Peak annotations to display the peak annotations that contain information for every peak on the chromatogram (Corresponds to pressing the icon). Press the Edit button (or the icon in the toolbar) in the Peak annotation screen to change the annotation content.
- Check Peak markers to display the markers that symbolize peak start and end (corresponds to pressing the icon . The colors of these markers can be modified (see below). Press the Customize button to change the peak markers style (cross, rectangle, triangle, circle.) and the size.
- Check Event annotations to display the integration events on the chromatogram at the time they are defined (Corresponds to pressing the icon). Press the Edit button (or the icon in the toolbar) to change their appearance in the Event annotations screen (see page 186).
- Check Event markers to display markers on the chromatogram at the times the integration events are defined (corresponds to pressing the icon). Press the Customize button to change the event markers style (cross, rectangle, triangle, circle) and the size.
- Check Baseline to display the baseline joining a Start and an End peak marker (corresponds to pressing the icon). Press the Customize button to change the baseline markers style (cross, rectangle, triangle, circle.) and the size.

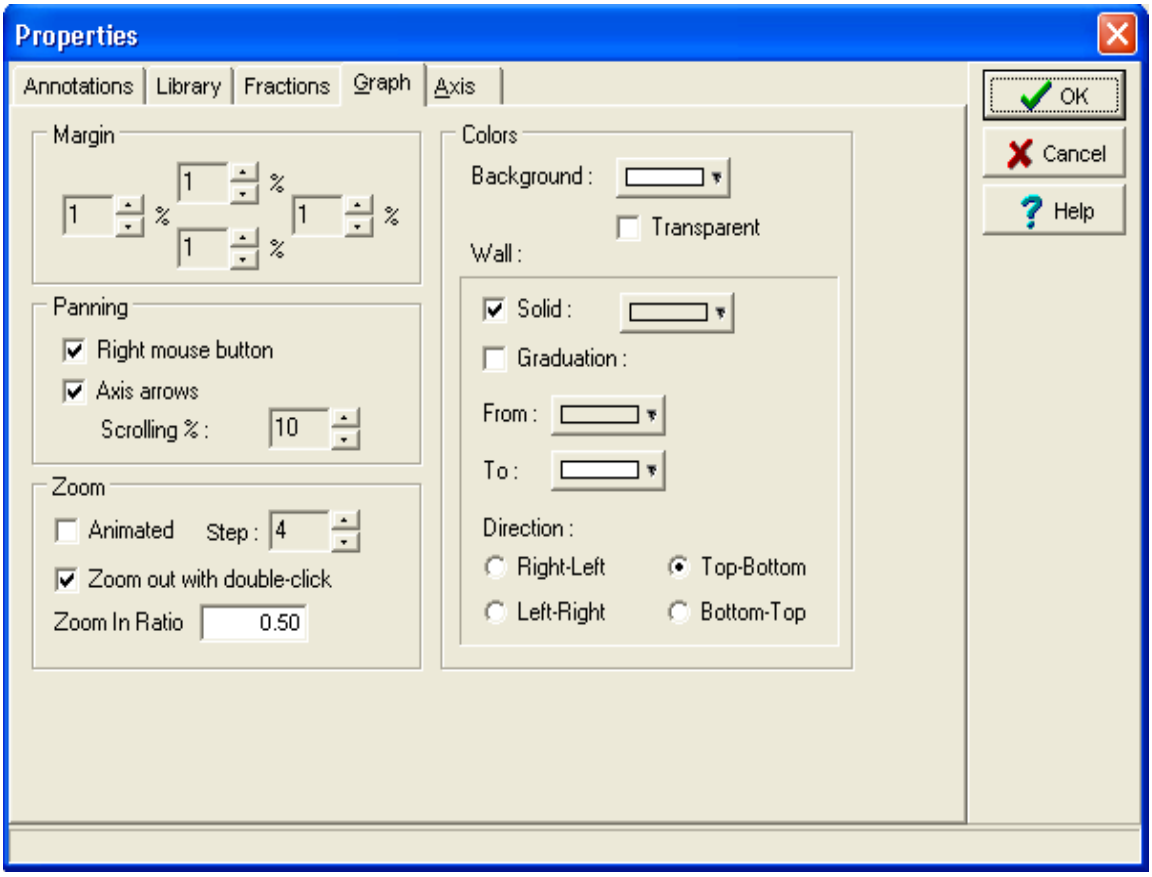
The colors of these markers can also be changed in this screen: start peak, stop peak, peak valley and event markers, including the baseline color.

The raw data color, the corresponding size and thickness of the plot can also be customized.

NOTE: The same screen is displayed from the chromatogram: Press the right mouse button within the chromatogram and select PROPERTIES in the popup menu or press the Chromatogram annotations icon .

Graph

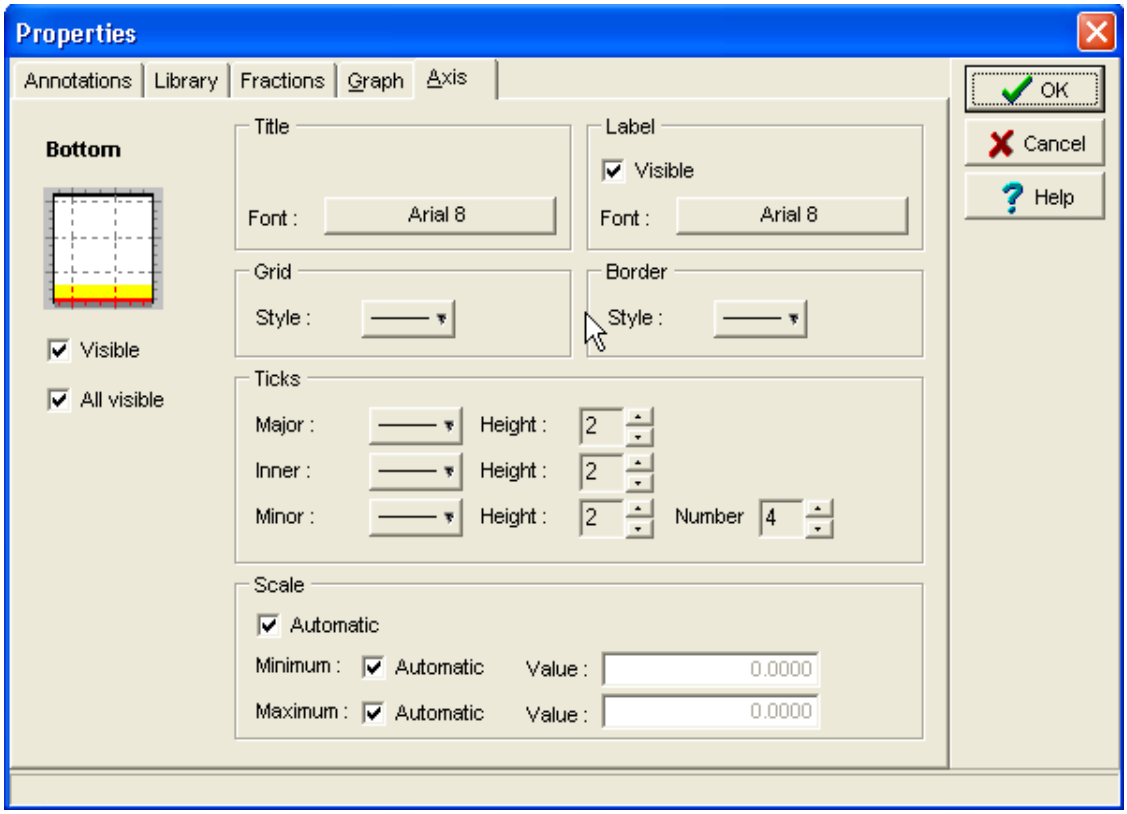
In the Curve properties, select the Graph tab.



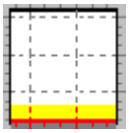
- In Margin Section, the interval between the curve and its border may be changed, as the percentages increase, the margin also increases.
- In Panning Section, check the box Right mouse button. Click and drag the right mouse button in the area of a graph, and the curve moves with the mouse (translation).
- Check the box Axis arrows. When the mouse is placed on an axis of the chromatogram, it takes the shape of an arrow. A left button click moves the curve in the arrow opposite direction. Change the % Scrolling value to choose the shifting length.
- Zoom Section: Check the box Animated to break down the zoom in as many steps as defined on the right of this check box.
- Check the box Zoom out with double-click, and the graph scale will be set as in the last zoom out action.
- The box Zoom in ratio is used to modify the speed of the zoom within the popup menu.
- Color Section: The background or frame colors can be changed by clicking on and then selecting the color of the background or the frame. Check graduation to obtain a graduated color effect for the graph frame.

Axis

In the Curve properties, select the Axis tab.



In the graph on the left, select (with a click) the axis to be configured:



The example above highlights the selected axis on the bottom (x-axis).

Now choose the parameters to configure the selected axis:

- Title:

Press the Font: Arial 8 button to select the font for the title of the curve.

- Label:

Press the Arial 8 button to select the axis font: the script, the height, the color, etc.

Uncheck the Visible box to hide the axis label.

Grid: Click on the arrow to modify the style of the graph grid and to show or hide it.

Border: Click on the arrow to modify the style of the graph border and to show or hide it.

Ticks: It is possible to modify the number of the ticks, their frequency, their length, etc.

The graphical properties are chosen only for the graph in which the right mouse button was pressed.

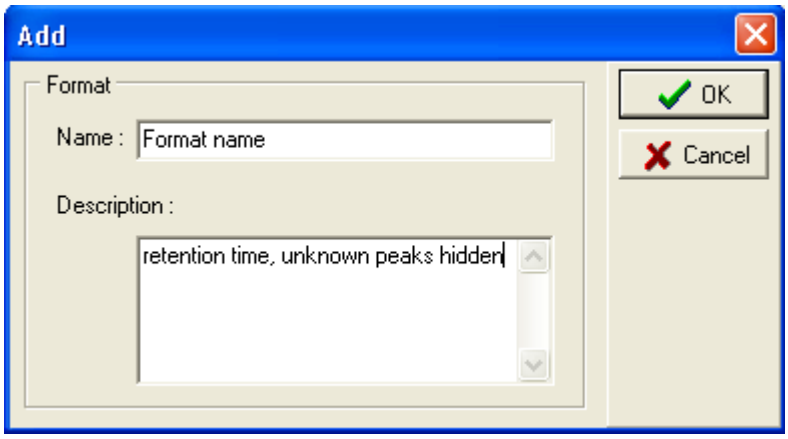
Library

Once chromatogram annotations and colors have been defined, it is possible to apply them for every new chromatogram. It is also possible to view the chromatogram with annotations, and then print it with a different set of annotations using the CompassCDS Report Editor. This is possible by using a saved chromatogram format.

The chromatogram annotations, graphic properties, and axis properties are saved in the chromatogram.

When all of these parameters are set correctly, the chromatogram format can be saved. In the chromatogram format, go to the ‘Library’ page and then press the ‘Save current format’ button.

Enter the name of the format in the window and a short description of the format in order to recognize it quickly:



Press OK and the format is added to all the other formats.

When a new method is defined, it is possible to apply an existing chromatogram format in the Format sub-method, press the ‘Edit’ button inside the chromatogram format, select ‘library’ tab in the corresponding format and apply it. To print the chromatograms with a special format, open the CompassCDS Report Editor, right click in the area of the chromatogram, select Properties, then select the name of the format in the top right hand corner of the window.

NOTE: The ‘Chromatogram name’ is always printed, whatever the corresponding option is checked or not in the library.

The Suitability Tests

The suitability tests allow the display of selected warnings if defined variables reach certain values. The tests can consider any variable available in the Variable editor (METHOD / VARIABLES).

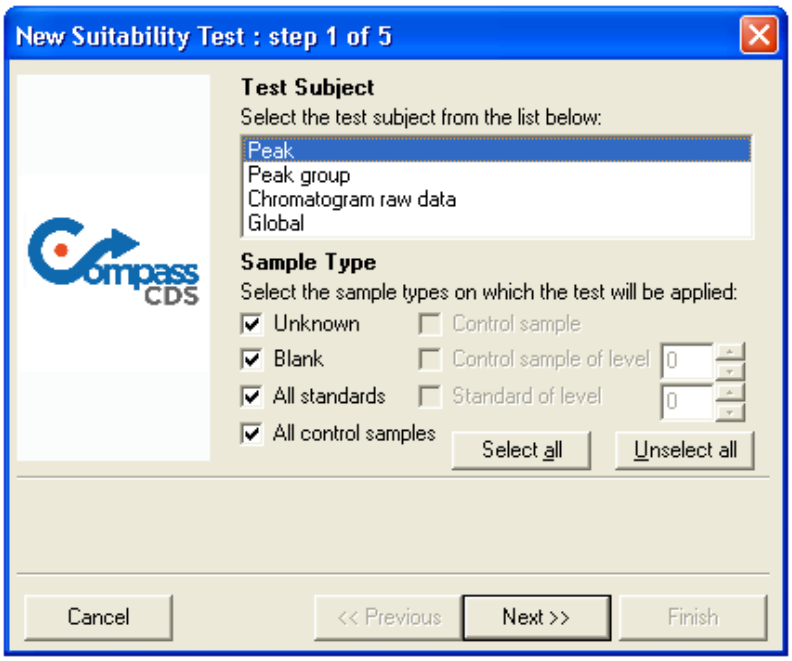
To display the suitability tests section of the method, select the menu METHOD / SUITABILITY TESTS or press the key combination Ctrl + T or select ‘Method’, then ‘Suitability’ in the browser.

Click on the Add button, then a 'Suitability test wizard' appears.

Suitability Test Wizard

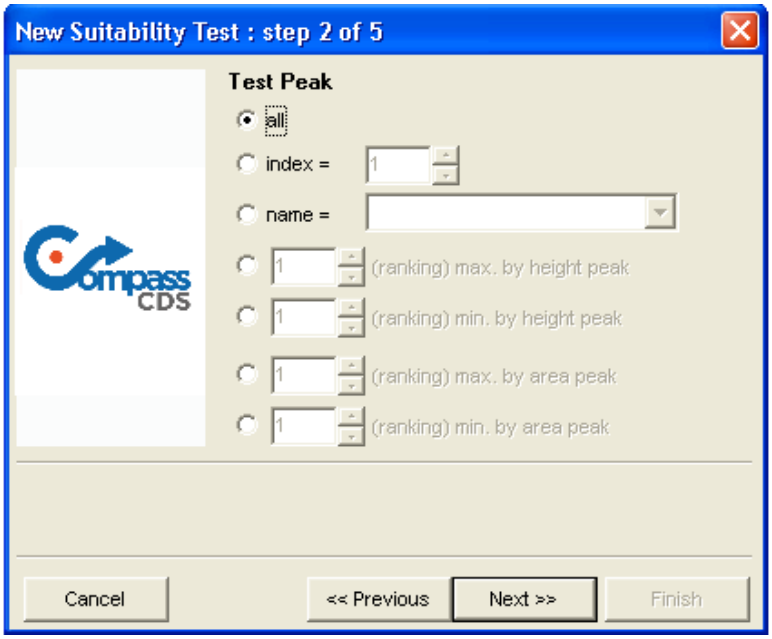
The wizard consists of several windows, which can be viewed using the NEXT and PREVIOUS buttons. When moving ahead within the wizard, text appears at the bottom of the screen, which lists what has been selected previously.

In the first window of the wizard, select the scope of the variable to be tested.



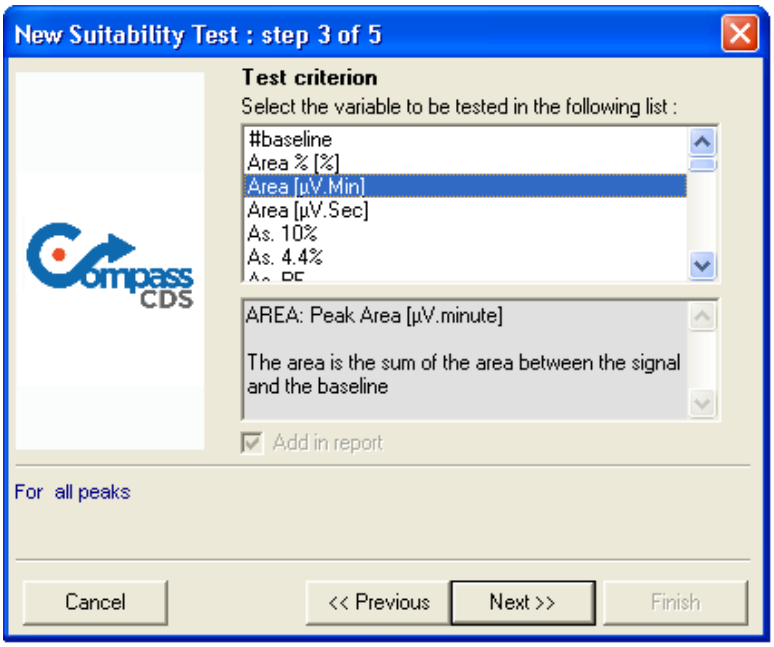
Choose to test either peak variables (quantity, area, asymmetry, etc.); or group variables (group quantity, group area, etc.); or chromatogram variables (sample mass, total area, etc., and all user input variables) or the chromatogram raw data (height of the signal). Precise the sample type concerned by the test: Unknown, blank, standard of a defined level or of all levels, control sample, control sample of a defined level or all control samples.

In the second window, choose the item to be tested.



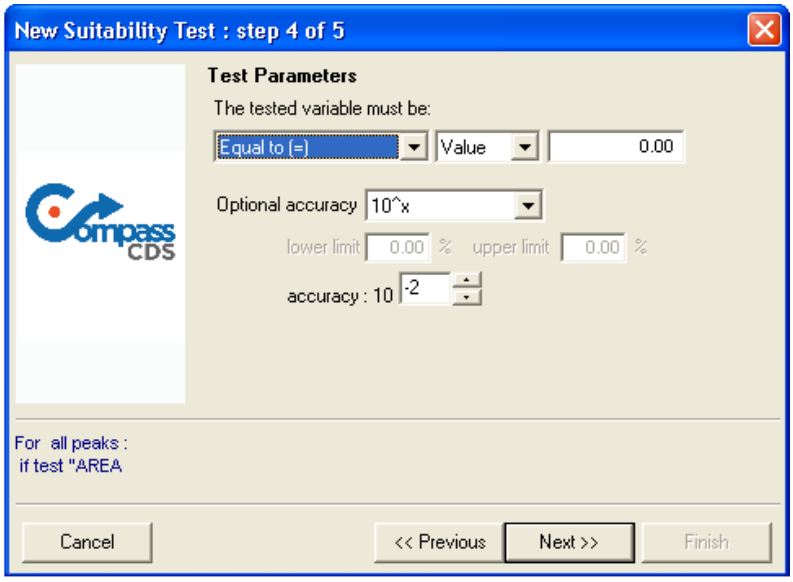
For example, if the tested variable is a peak or a group variable, choose if all the peaks or all the groups should be tested or choose the name, the index, etc., of the peak or group that should be tested. If the signal value is tested, choose which acquisition points (slice) must be tested: all the points (whole); the points between the x^{th} and the y^{th} acquisition points (Slices from x to y); or the points between x and y minutes (Time range from x to y min). If the variable is a global one (chromatogram variable) then this step is by-passed.

In the third window of the wizard, the tested variables are chosen:



The list of all the variables defined for the selected scope is displayed, including the user defined variable. Click on the variable to be tested and press the Next button. If the signal value is tested (raw data), choose to test either the minimum value of the signal between the two limits or the maximum value.

In the fourth step, choose the second part of the test.



The variable(s) can be defined as equal or different to a certain value or of another variable value, with a precision. The variable(s) can also be defined greater than or less than a certain value (strictly or not).

“Optional accuracy” settings:

Computers cannot handle precisely. Indeed there are some fractional values that cannot be represented at all, and if a calculation results in one of those numbers, then the result is the nearest Real number that it can provide. Which numbers those are depends on the precision of the number used.

CompassCDS uses Double precision but technically absolute accuracy is not possible. So, rather than an option of equality, one should really say “equal to or at least very near to” when dealing with Real numbers, which is exactly what “Accuracy” does, it give a small amount of lee-way in the equality check.

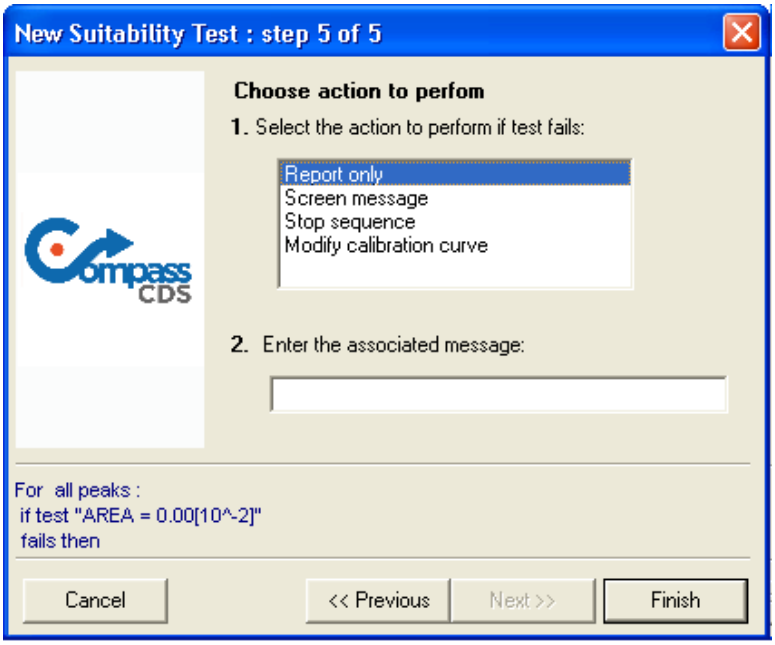
So, in the above setting the QTY of “Peak A” must be equal to 10.0, or at least within 10-2 of 10.0, i.e., 9.99 to 10.01. To increase the accuracy scroll the accuracy control to a more negative number.

This topic originally arose due to the desire to use a control sample to check the calibration. In this scenario one wouldn’t expect exactly the nominal value, but something close to it. Also, the above case presumes the desired value is in the middle of the allowed range, and this is not always the case. This is when the alternative setting of “Limits” can be used.

As can be seen, different lower and upper limits can now be set, as a percentage of the target value.

So in the above case, if the calculated concentration of any peak is within 99% to 102% of the defined level in the Control standard, the test will have deemed to have been passed, if the concentration is outside these limits, it will have failed.

In the last step, choose the action to perform if the test fails.



The user can define a message to display only in the printed report (Report only), or both in the printed report and on the screen (Screen message). The user can also decide to stop the sequence after the processing of the current chromatogram acquisition by choosing the 'Stop sequence' option. This option has a meaning only for suitability done during a sequence run. The Modify calibration curve action has to be used only if 'Control sample of level' is selected to realize the test. The action is that if the test failed all the calibration points of the same level than the one of the 'Control sample of level' that is tested are removed from the calibration curve and replaced by the unique point corresponding to the 'Control sample of level'.

By default, if a test is done on all the peaks, a new variable which result is either true or false is created. This variable can be displayed in the peak report. The name of this variable is SuitabilityX and it is possible to rename it in the variable editor. In the same way a group variable is created if a test is done on all the groups.

Press 'Finish' button in the last window to add the test. When the test is added, select it and press the button 'Edit test' or 'Edit action' to modify the test.

Suitability Test Examples

- **Peak asymmetry:** To test the peak asymmetry, add a suitability test. Choose Peak as the test subject, choose to test "All" peaks, choose As10% as the test criterion, choose between 0.9 and 1.1 as the test parameters. Then choose Report only as the result and press 'Finish'. In the peak report press the right-mouse button and choose Report properties and add a column for the suitability test.
- If you want to change the heading of the column, select the menu METHOD / VARIABLES. Search for the variable called 'Suitability 1' corresponding to the test and change the name to 'Asymmetry'.
- **Quantity of a component:** To test the quantity of a component (e.g. Benzene), add a suitability test. Choose Peak as the test subject, choose to test a peak selected with its name and select Benzene from the drop-down list, choose Qty as the test criterion, choose less than 15 as the test value. Then choose Report only as the result and enter a message saying 'Quantity of Benzene is superior to 15 ppm' for example and press OK. Now, in the

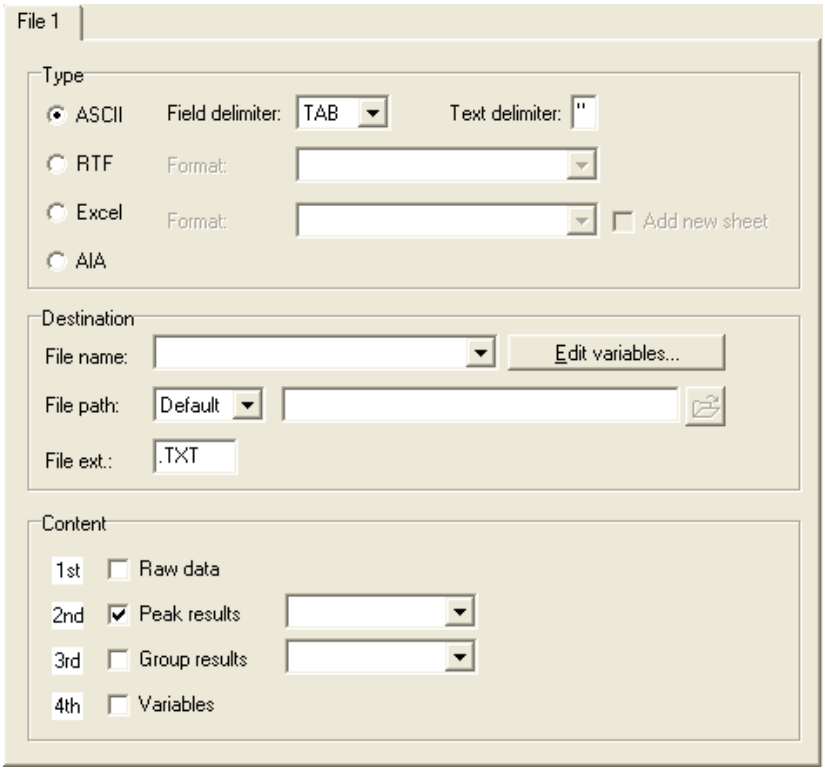
report style in the CompassCDS Report Editor, Add a Suitability result object to print the alarm if the test is negative.

To add a suitability test object in the CompassCDS Report Editor, press

Exporting the Results

It is possible to automatically export certain data (chromatogram, peak report or group report) in a defined format (Word, Excel, AIA, ASCII).

In the export section of the method, press the Add button and the following screen is displayed:



First choose the file type in which the results are to be exported: ASCII, Excel, AIA, or RTF

- **ASCII:** Choose the field delimiter that will separate the elements contained in a table. By default it is a tab, but choose “other” to delimit the text with any other character. Choose also the text delimiter that will enclose text fields.
- **Excel:** Select the version of the Excel program that will use the exported file.
- **AIA:** Export of level 3. This export contains raw data (point number, rate, etc.); peak data (result table, method name, peak variables, etc.); detection method parameters; sample description (mass, injection volume, information, etc.); administrative data (operator, data set origin, chromatogram title, etc.).
- **RTF:** Select the application in which the exported file will be read.

Then choose the file destination:

- **Name:** The name of the file can correspond to a variable. For example, choose Chromatoname from the list and the name of the exported file will have the name of the chromatogram with the chosen extension.

A special variable can be created to specify the file name. For example, click on ‘Edit variables’ and, within the Variable editor, create a new variable called ‘ExportName’. For example purposes, it will be a global variable, a string, defined with the following user formula: ‘Export_’+Chromatoname’. Now press the Apply button and select ExportName in the File name list box. In this case, if the chromatogram is called “chromato_1.data”, the name of the exported file will be “Export_ chromato_1.ext”.

To export a file for each channel when there are several channels in a method, define a variable whose formula will be ‘Chromatoname+Channelnumber’.

If variables have the same value in different chromatograms, the results can be exported to the same Excel file but in different worksheets. Check the box ‘Add new sheet’ in the export part of used method.

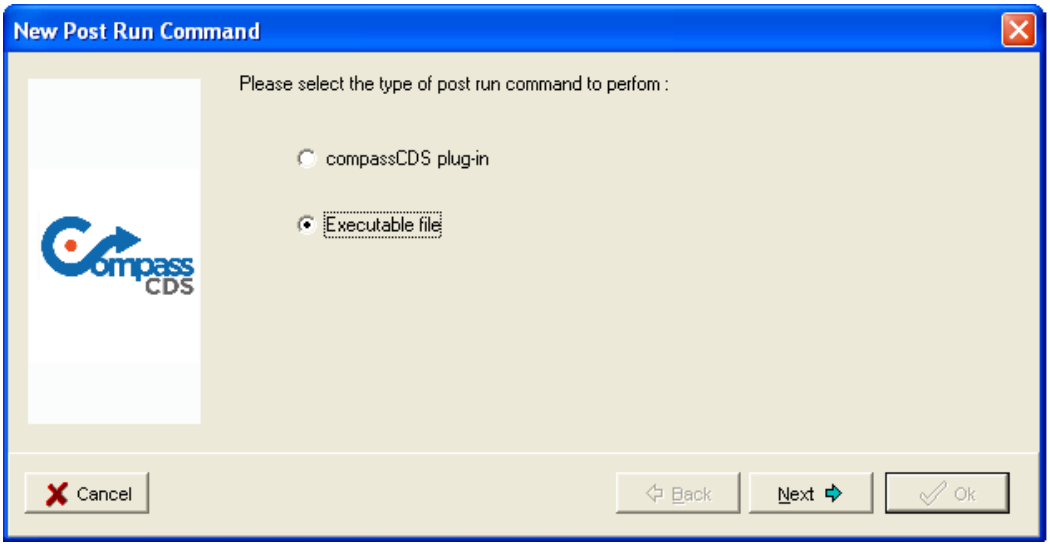
- **Path:** Choose the path of the directory in which the file will be exported. By default, the path will be the chromatogram path, but, if the Custom option is chosen from the drop list box, another path can be defined in next field.
- If the entered path does not exist, it is created during processing.
- **Extension:** By default, an extension corresponding to the file format will be defined, but it is possible to change it, e.g. defining a special format for a LIMS.
- Now choose the content of the exported file:
- **Raw data:** Check this box to export the raw data (the retention time and the absolute height of each point of the chromatogram). The raw data is always exported in the case of AIA export.
- **Peak results:** Check this box to export a peak table, which is the list of the chromatogram peaks. To define the format of this table, select the format of the peak table in the associated scrolling list (formats are created and detailed page 95). In case of AIA export, the format will be exported as it is defined in the current chromatogram results table
- **Group results:** Check this box to export a group table (the list of the groups). A format for this table may also be specified (as for peak results).
- **Variables:** Check this box to export all the global variables (the list of the global variables with their values).

Be careful to close the file before executing the processing. If the export file name is always the same and if you open it and start the processing, the export cannot be completed. In addition, if a file with the same name already exists, it will be overwritten without a warning message.

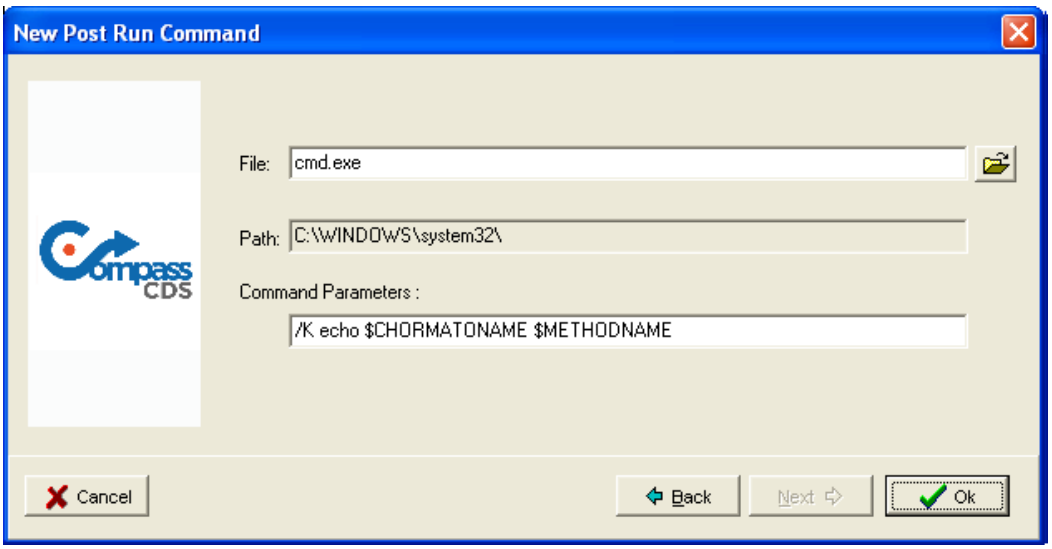
The Post Processing

This function allows the automatic execution of a program (Plug-In) using CompassCDS results.

Click on the add button, and then specify in the following screen whether the post processing is a plug in or an executable file.



If it is an executable file, the following screen is displayed:



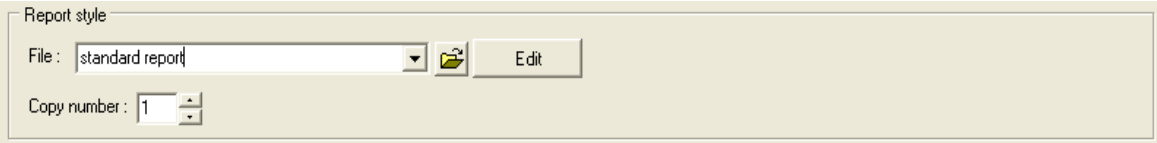
Select the executable file name in the ‘File’ field, the path is automatically displayed in the ‘Path’ field.

If the program to run needs some CompassCDS global variable(s) (system or user input variables) to be executed, the user has to define these variable names in the command parameters field. The syntax to use is ‘$’ and the ‘variable name’ (refer the variable chapter to know the name of the variables): $VARIABLEID1 $VARIABLEID2 etc.

According to the executable file chosen, a particular syntax can be used (see the example using the prompt command program where ‘/K echo’ is used to let the command prompt window open after the post processing has been executed.

Report Printing

The section ‘Report Style’ allows the user to define report printing. The following screen is displayed:



In the “File” box, select the name of the report template to print. Some templates must first be created in the CompassCDS Report Editor (see the corresponding user’s guide manual).

To view the selected report, press the Edit button: CompassCDS Report Editor is opened and displays the corresponding report template.

To print automatically a report after an acquisition, enter 1 in the “copy number” box. If 0 is selected, no printing will be done automatically.

The Summary Report

This function allows the user to generate a statistical report. All variables defined in CompassCDS can be statistically followed over time (retention time, RF, area, etc.). This is useful, e.g. for following column ageing by plotting the standard deviation of the retention time of a compound under specified analytical conditions.

This function is described in detail beginning on page 194.

Method Templates

Once a method has been built, it is possible to save it as a model in order to reuse it for the creation of new methods associated with other systems.

The methods created from a method template are the same as the original one except that the control section is not transferred.

Creating a Method Template

Once a method is created and saved, it is possible to save it as a template: Select this method and then the FILE / SAVE AS / SAVE METHOD AS TEMPLATE menu.

Now, you need to specify a name for the template method, be sure to enter a description of the template method in the corresponding field because this description will help you to identify it in the Open File window.

All the parameters of the mother method are saved in the template method, except the control parameters.

Creating a New Method using a method template

Select the menu FILE / NEW / NEW METHOD FROM TEMPLATE. Select the name of the template you would like to use and then select the system (chromatograph) the method should be applied to. A new method is created, using the model of the method template and with the default control parameters associated with the selected system.

This method can be manipulated as if it is a newly created one.

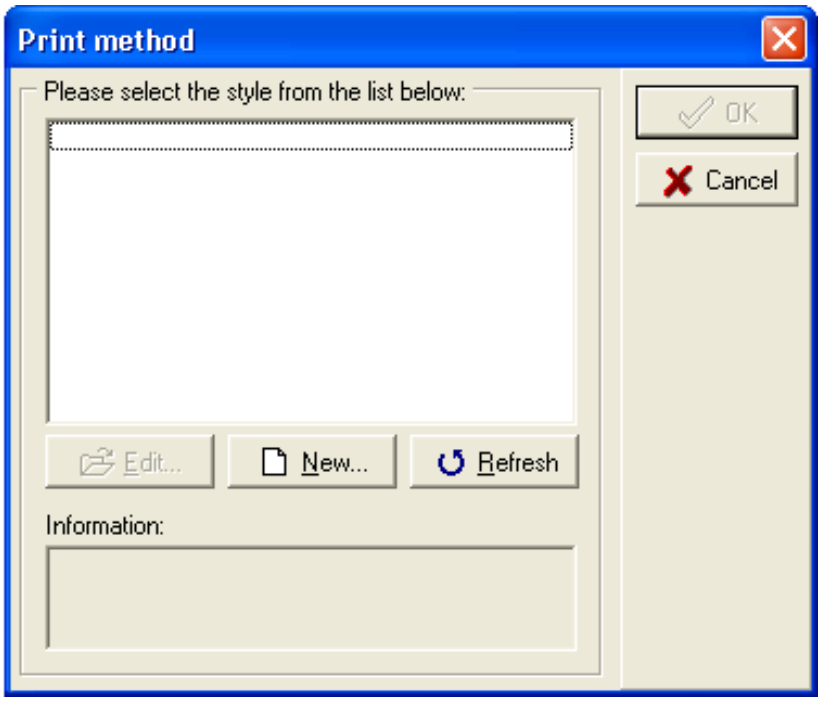
Do not forget to enter the parameter values in the control section.

Template Method Path

The templates methods are saved in a specific path, common to a group. This path is specified in the CompassCDS Configuration Manager and can be different from the data path.

Printing Method Parameters

To print method parameters, open it, and then click on the icon. The following screen is displayed:



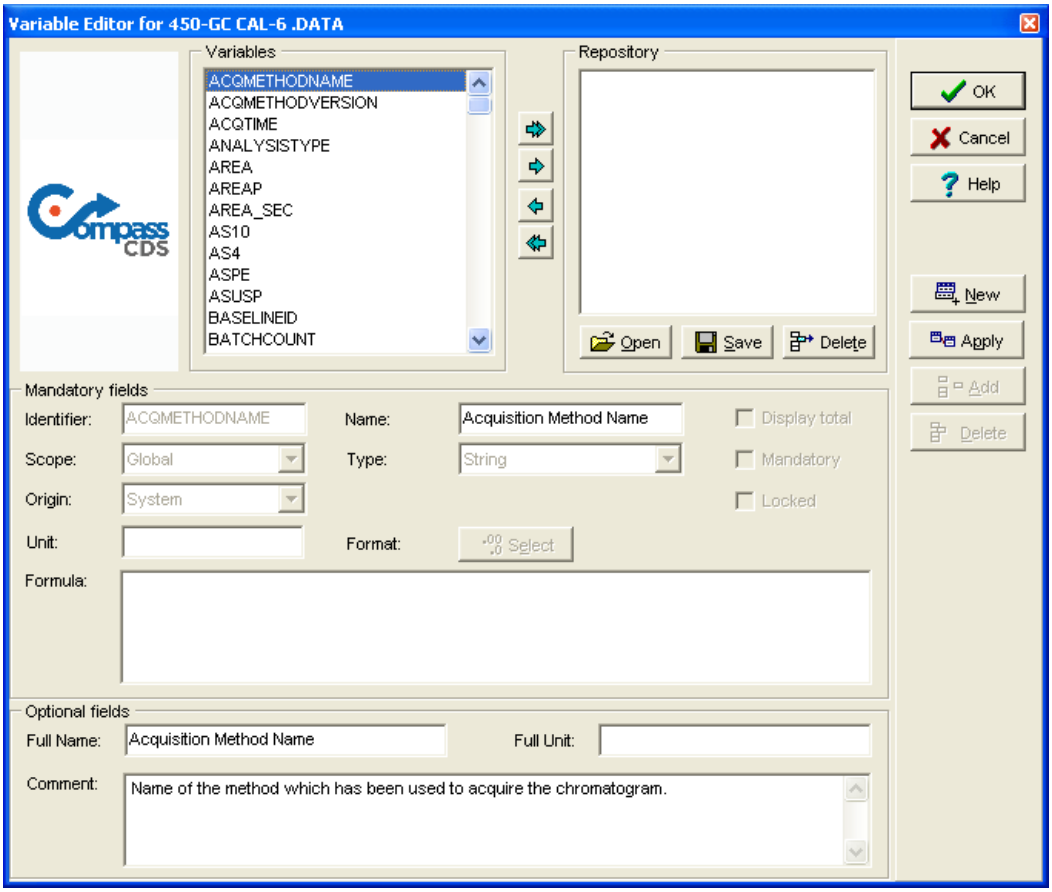
When the user selects a defined report in the list, he can edit it by pressing the Edit button; create a new one by pressing the ‘New’ button to customize the report, or refresh the list by pressing the ‘Refresh’ button.

CompassCDS Variables

CompassCDS incorporates many system variables that can perform calculations on individual peaks, peak groups, or the entire sample. It can also offer the possibility to define custom variables for calculations, which are not present by default in the existing CompassCDS variables. These can be either ‘user input’ variables for which the user must enter a value or text, or ‘user formula’ variables which allow specific calculations.

The variables are saved as part of the current method.

The management of the variables is done in the CompassCDS Variable Editor, available from the METHOD / VARIABLES menu:



The Variable Editor is composed of several parts, detailed in this manual:

- Variable list
- Repository
- Variable definition parameters

And specific buttons:

New: Creation of a new variable

Apply: Apply the changes made for the selected variables

Add: Save a variable with another name (remind to change the identifier)

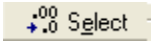
Delete: Delete the selected non-system variable

How a Variable is Defined

A variable is defined by the following elements:

- **Identifier:** The identifier is a short name to identify the variable. It can be used to print the variable in the CompassCDS Report Editor or be used to insert the variable into the formula of another variable. An identifier must be composed of letters, numbers or underscores. The first character of an identifier should be a letter.
- **Name:** The name of the variable is used to identify the variable into the software. For peak variables, the name is used in the peak result table (column heading), and also in the peak

results object in the CompassCDS Report Editor reports. For group variables, the name is used in the group report. For global variables, the name is used in the CHROMATOGRAM PROPERTIES. The name of the standard variables can be modified.

- **Unit:** The abbreviation of the unit of the variable. It is indicated in the heading of the peak or group report, or in the CHROMATOGRAM PROPERTIES after the name of the variable. The unit of standard variables can be modified.
- **Scope:** The scope is used to define if the variable applies to a peak, peak group, or the entire sample. For example, Area and Quantity can apply to peaks or groups, and sample weight is global. Peak variables can be displayed in the peak report; group variables can be displayed in the group report, while global variables are displayed in chromatogram properties (menu options DATA / CHROMATOGRAM PROPERTIES).
- **Type:** The type of a variable can be a real number, an integer, a string of characters or Boolean. A Boolean is defined by a condition in a formula (see below). If the condition is satisfied, the value of the Boolean is TRUE, otherwise, it is FALSE. It is possible to modify the type of a variable. To transform a real into an integer, use 'Trunc' or 'Round'. To transform a string into a real, use 'Float'. To transform a real into a string, use 'String' (see the 'Usual Functions' chapter, page 134).
- **Default value:** This field is accessible only for non-mandatory user input variables ('global' and 'by peak'). It allows entry of a default value.
- **Origin:** The origin of a variable depends on the way in which the value of the variable is obtained. For a standard variable, the origin of the variable will be 'System'. User- defined variables can be calculated with a formula ('User formula'). The user can also edit them in the acquisition windows (Quick Start or sequences) or in the CHROMATOGRAM PROPERTIES if the origin is 'User input'.
- **Display total:** This box is active only for group and peak variables. Check this box if the variable is to be summed for all the peaks or groups. The total will appear at the bottom of the peak or group report.
- **Mandatory variables:** This box is active only for 'User input' variables. By checking this box, CompassCDS will refuse to launch an acquisition if the variable has not been entered (in Quick Start window or the sequence).
- **Locked:** This option is available only if the user owns the corresponding profile. The user input variable may be locked so other users may not change it.
- **Format:** Press the Format button 

to define the display format of the real numbers. Three types of formats exist: automatic, scientific, and fixed. Choose the number of decimals to be displayed. For example, for the area variable, select scientific with a precision of 5, and the area of a peak displayed will be '4.18345e4'. If fixed is selected with a precision of 3, the same area will be displayed as '4183.452'. Automatic mode is the same as fixed mode, but with comma separation at each thousand. The format may be modified for standard variables.
- **Formula:** This field is accessible only for User formula variables. It allows the definition of the calculation formula of the variable (see the' How to Express the Formula' chapter, page 131).
- **Full name:** The full name of the variable is given in this area. This full name appears only in this window. It provides information related to the content of the variable.
- **Full unit:** The full name of the unit is given in this area. This full unit appears only in this window. It provides information related to the unit of the variable.
- **Comment:** A comment that explains the calculations of the variable, its origin, or any other useful information. This information cannot be modified for system variables.

For the system variables, it is only possible to modify the full name and the format.

System Variables

The system variables are defined by default in CompassCDS. As mentioned in the previous paragraph, a variable is defined by an Identifier and a Name. In this section, all the system variables are described and listed by their Name and Identifier under the following syntax: Name [IDENTIFIER].

Peak System Variables

The peak system variables can be displayed in the peak report. (Choose REPORT FORMAT in the popup menu and select the variables for report display).

CompassCDS calculates the following variables automatically for each peak:

Retention Time

- **Corrected time** [min**] [RTCORRECT]:** Theoretical retention time (from the identification table) corrected according to the retention times of reference peaks. For example, if a peak was expected at 9 minutes between two reference peaks expected at 8 and 10 minutes, and the reference peaks occur at 8.5 and 10.5 minutes, the corrected retention time of the peak will be 9.5 minutes (See “Identification” section).
- **RT. Index [RTINDEX]:** This is an index giving the position of the peak between the two adjacent reference peaks: If the two adjacent reference peaks are the nth and the n+1th reference peaks, the RT index of the peak equals:

$$\text{index} = \frac{\text{Rt} - \text{Rt}_n}{\text{Rt}_{n+1} - \text{Rt}_n} + n$$

Where

Rt is the peak retention time.

Rtn is the retention time of the previous reference peak.

Rt_{n+1} is the retention time of the next reference peak.

- **RT Offset** [min] **[OFFSET]:** This parameter is calculated for identified peaks and is the difference (in minutes) between the theoretical retention time of the peak and its actual retention time. The theoretical retention time is the time set in the identification table.
- **Start** [min] **[RTSTART]:** Time at the beginning of the peak (in minutes). It corresponds to the time of the peak start marker (or if the marker is a valley).
- **Stop** [min] **[RTSTOP]:** Time at the end of the peak (in minutes). It corresponds to the time of the peak stop marker (or if the marker is a valley).
- **Time** [min] **[RT]:** Retention time at the peak apex (in minutes).

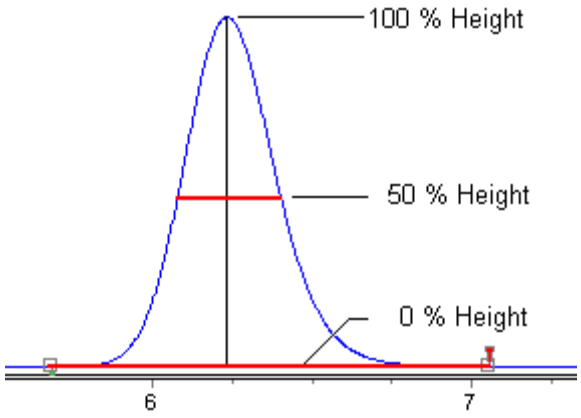
Response

- **Area** [µV.min] **[AREA]:** The area is the sum of the area between the signal and the baseline between the two peak edges (peak start and end markers).
- **Area** [µV.sec] **[AREA]:** The area is the sum of the area between the signal and the baseline between the two peak edges (peak start and end markers).
- **Area** [%] **[AREAP]:** The area percentage is the area of the peak divided by the sum of the areas of all the peaks, multiplied by 100.

- **Height** [µV] **[HEIGHT]:** The height is the difference between the value of the signal at the apex of the peak and the value of the baseline at the same time.
- **Height** [%] **[HEIGHTP]:** The height percentage is the height of the peak divided by the sum of the heights of all the peaks, multiplied by 100.
- **Recomputed RF [RF_Rec]**: This is the recomputed response factor. It is equal to the ratio between the quantity calculated by CompassCDS and the response.
- **Recomputed RRF [RRF_Rec]:** This is the recomputed inverse response factor. It is equal to the inverse of the Recomputed Response Factor.
- **Response [RESP]:** The response is either the area, the height, the area% or the height%, the area$^{1/2}$ and the height$^{1/2}$ according to the choice made in the calibration method (response section).
- **RF [RF]:** This is the response factor entered in the calibration table (in the case of a calibration with manual response factors) or the ratio of the quantity (read from the calibration curve) of the peak by its response (in the case of calibration with a calibration curve).
- **RRF [RRF]:** This is the inverse response factor. RRF = 1/RF= Response / Quantity.

Width

- **Width X%** [min] **[WX]:** The width of the peak measured at the specified height (X). The height is expressed as a percentage of the total height of the peak. 0% of the height is on the baseline, 100% of the height is on the top of the peak:



A height of 4.4% corresponds to the 5-sigma method

A height of 13.4% corresponds to the 4-sigma method

A height of 32.4% corresponds to the 3-sigma method

A height of 60.7% corresponds to the 2-sigma method

Seven heights are proposed:

X= 4 means 4.4 %

X= 5 means 5 %

X= 10 means 10 %

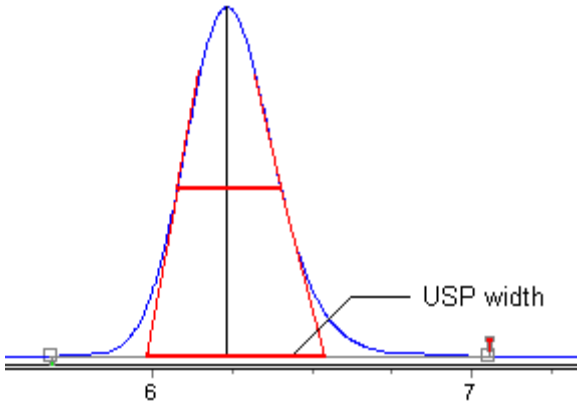
X= 13 means 13.4 %

X= 32 means 32.4 %

X= 50 means 50 %

X= 60 means 60.7 %

- **Width USP** [min] **[W_USP]:** Peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.



- **Left Half Width X%** [min] **[WLX]:** Left half peak width measured at the specified height (X).The height is expressed as a percentage of the total height of the peak. 0% of the height is on the baseline, 100% of the height is on the top of the peak:

Seven heights are proposed:

X= 4 means 4.4 %

X= 5 means 5 %

X= 10 means 10 %

X= 13 means 13.4 %

X= 32 means 32.4 %

X= 50 means 50 %

X= 60 means 60.7 %

- **Left Half Width USP** [min] **[WL_USP]:** Left half peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.

Asymmetry

- **As.PE. [ASPE]:** Asymmetry calculated with the European Pharmacopoeia method:

$$A_s = \frac{W_{5\%}}{2 * W_{1/2}}$$

Where

W5% is the peak width at 5% of peak height.

W1/2 is the first half-width at 5% of peak height.

- **As.USP. [ASUSP]:** Asymmetry calculated with the United States Pharmacopoeia method:

$$A_s = \frac{W_{5\%}}{2 * f}$$

Where

W5% is the peak width at 5% of peak height.

f is the first half-width at 5% of peak height.

- **As.EMG/ASTM [ASUSP]:** EMG and ASTM methods for Asymmetry calculation are the same as the United States Pharmacopoeia method.
- **As. 4.4% [AS4]:** It is a half-width method:

$$A_s = \frac{W_{2/2}}{W_{1/2}}$$

Where

W1/2 is the first half-width at 4.4 % of peak height.

W2/2 is the second half-width at 4.4 % of peak height.

- **As. 10% [AS10]:** It is a half-width method:

$$A_s = \frac{W_{2/2}}{W_{1/2}}$$

Where

W1/2 is the first half-width at 10 % of peak height.

W2/2 is the second half-width at 10 % of peak height.

Number of Theoretical Plates

- **NTP Sx [NTP_SX]:** This is the number of theoretical plates calculated with the x-sigma method:

$$NTP = R_{sigma}\left(\frac{R_t}{w}\right)^2$$

Where

Rt is the peak retention time.

w is the peak width at the height corresponding to the calculation method:

R_{sigma} is a factor which depends on the calculation method:

5 sigma method: R_{sigma} = 25, width measured at 4.4 % of peak height

4 sigma method: R_{sigma} = 16, width measured at 13.4 %

3 sigma method: Rsigma = 9, width measured at 32.4 %

2 sigma method: Rsigma = 4, width measured at 60.7 %

- **NTP USP [NTP_USP]:** This is the number of theoretical plates calculated with the United States Pharmacopoeia method:

$$NTP = 16 \times \left(\frac{R_t}{w} \right)^2$$

Where

Rt is the peak retention time

w is the USP Width (peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.)

- **NTP EP [NTP_EP]:** This is the number of theoretical plates calculated with the European Pharmacopoeia method:

$$NTP = 8\mathrm{Ln}(2)\left(\frac{R_t}{w} \right)^2$$

Where

Rt is the peak retention time.

w is the peak width measured at the half peak height.

- **NTP JP/ASTM [NTP_EP]:** JP and ASTM methods for theoretical plate's number calculation are the same as European Pharmacopoeia method.
- **NTP EMG [NTP_EMG]:** This is the number of theoretical plates calculated with the EMG method:

$$NTP = 41.7 \times \frac{\left(\frac{R_t}{W_{10\%}} \right)^2}{\frac{W_{1/2-10\%}}{W_{2/2-10\%}} + 1.25}$$

Where

Rt is the peak retention time

W10% is the peak width measured at 10% of peak height.

W1/2-10% is the first half peak width measured at 10% of peak height.

W2/2-10% is the second half peak width measured at 10% of peak height.

- NTP AH [NTP_AH]: This is the number of theoretical plates calculated with the Area/Height method:

$$NTP = 16 \times \left(\frac{R_t}{4 \times 0.399 \times \left(\frac{A}{h} \right)} \right)^2$$

Where

Rt is the peak retention time

A is the area of the peak in µV.min.

h is the height of the peak in µV.

Selectivity, Capacity

- **α[SEL]:** This is the selectivity factor, which is the ratio of the peak capacity factor (k') to the capacity factor of the previous peak:

$$\alpha = \frac{k_2}{k_1} \quad \text{or} \quad \alpha = \frac{Rt_2 - T_0}{Rt_1 - T_0}$$

Where

T_0, Rt_1 and Rt_2 represent respectively the dead time, the peak retention time of the previous peak and the retention time of the current peak.

The dead time, T_0, set in the acquisition window (Quick Start or sequence), can be modified in the chromatogram properties (Menu DATA / CHROMATOGRAM PROPERTIES).

- **k' [KP]:** the capacity factor (k') of a compound is the ratio of the quantities of the compound in the stationary phase and in the mobile phase.

$$k' = \frac{Rt - T_0}{T_0} = \frac{qstat}{qmob}$$

Where

T_0 and Rt represent respectively the dead time and the peak retention time, qstat the quantity of the compound in the stationary phase and qmob the quantity of the compound in the mobile phase.

Resolution

The resolution quantifies the integrity of the separation between two successive peaks.

- **Res. HW [RES_HW]:** This is the resolution calculated with the half width method:

$$R_s = 1.18 \times \frac{Rt_2 - Rt_1}{W_1 + W_2}$$

Where

Rt_2 and Rt_1 represent respectively the peak retention time and the retention time of the previous peak.

W_1 is the half height width of the first peak.

W_2 is the half height width of the second peak.

- **Res. EMG/EP/ASTM [RES_HW]:** EMG, European Pharmacopoeia, and ASTM resolutions are calculated as half width Resolution.

- **Res. USP [RES_USP]:** This is the resolution calculated with the United States Pharmacopoeia method:

$$R_s = 2 \times \frac{Rt_2 - Rt_1}{w_1 + w_2}$$

Where

Rt_1 and Rt_2 represent respectively the peak retention time of the previous peak and the retention time of the current peak.

W_1 is the USP width of the previous peak.

W_2 is the USP width of the current peak.

See the section on Peak width for how USP width is calculated.

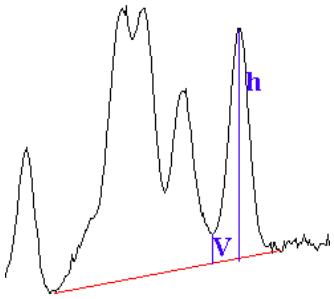
- **Res. Val. [RES_VAL]:** This is the resolution calculated with the valley method:

$$R = \frac{V}{h}$$

Where

V is the height of the valley preceding the peak.

h is the height of the peak.



Name, Quantities

- **Control sample [CTRLSAMPLE]:** It is the quantity entered in the calibration table for the control sample. This value is used for the control sample computation.
- **Name [NAME]:** The name assigned to the peak after the identification (See “Identification” section). The name is used to quantify the peak if the calibration mode is different from response percentages.
- **Qtable [QTABLE]:** Quantity entered in the calibration table for the peak and the corresponding chromatogram level, if the chromatogram is a standard or a control sample with level.
- **Quantity [unit] [QTY]:** The quantity of the peak (See Quantification section).

Integration Code [CODE]

The integration code describes the way in which the baseline is drawn. The first letter describes the baseline position at the peak start and the second letter the baseline position at the peak end.

Possible cases:

S The baseline is on the signal.

H The baseline is horizontal.

V The end or the start of the peak is a valley.

T The peak is a shoulder, the baseline is tangential.

E The peak is a shoulder, the baseline is exponential.

M The peak has been integrated manually.

F The end or the start of the peak has been forced.

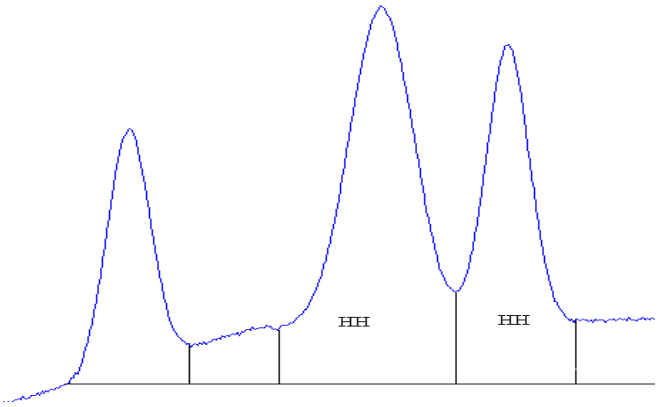
OR When the peak is saturated (Out of Range).

Priority rules:

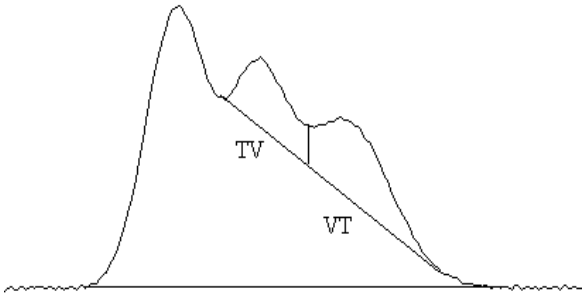
1. H has priority over S and V.
2. E and T can be replaced by V.
3. F has priority over H, S, V.
4. M has priority over F, H, S, V, E and T.
5. E and T have priority over S.
6. OR has priority over F, H, S, V, E and T.

Integration examples:

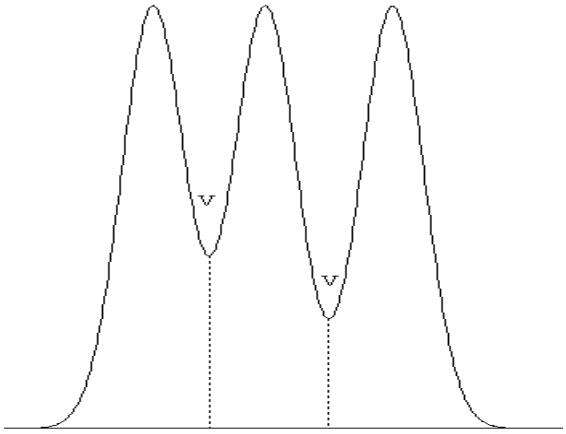
1. The baseline has been forced (rule 1).



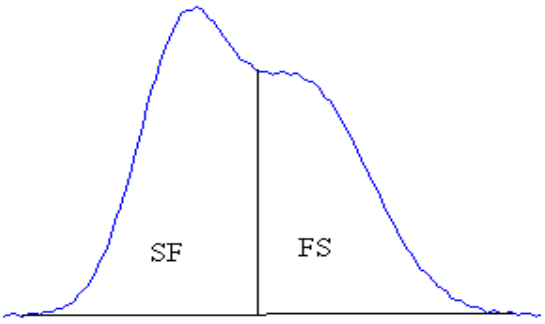
2. Two peaks integrated as tangential shoulders of a main peak (rule 2).



3. Integration ‘Valley to Valley’.



4. Forced integration: split peak.



It is also possible to indicate the saturation of a peak thanks to this variable. The associated code is OR (out of range). User has to enter the minimum and maximum value of the output signal (of the chromatograph) in the METHOD / INTEGRATION / PARAMETERS menu.

Saturation

Saturated [ISSAT]: This variable displays TRUE if the corresponding peak is saturated, FALSE in the other case according to the minimum and maximum values of the output signal (chromatographic signal) defined in the METHOD / INTEGRATION / PARAMETERS menu.

Moments, Excess (or Kurtosis), Skew

- **Moment1 [MOMENT1]:** The first moment of a peak is the mean retention time, which is the retention time of the peak at the center of gravity. It is referenced to the peak retention time (m1 is the time between the top and the center of gravity of the peak).

$$m_1 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)h_t dt$$

Where

m0 is the zero moment, or the peak area.

Rt the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

In the case of a Gaussian peak, m1 is equal to zero.

- **Moment2 [MOMENT2]:** The second moment of a peak is the variance 2σ (σ is the peak standard deviation). The second moment is a measure of the lateral spread.

$$m_2 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^2.h_t dt$$

Where

m_0 is the zero moment or the peak area.

R_t is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

- **Moment3 [MOMENT3]:** The third moment of a peak describes vertical asymmetry, or skew. It is a measure of the departure of the peak shape from the Gaussian standard.

$$m_3 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^3.h_t dt$$

Where

m_0 is the zero moment or the peak area.

Rt is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

In the case of a Gaussian peak, m_3 is equal to zero.

- **Moment4 [MOMENT4]:** The fourth moment (or excess) of a peak is a measure of the compression or stretching of the peak along a vertical axis, and how this compares with a Gaussian standard.

$$m_4 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^4.h_t dt$$

Where

m_0 is the zero moment, or the peak area.

Rt is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

- **Excess or Kurtosis [KURTOSIS]:** Excess is equal to zero for Gaussian peaks. E is negative for overloaded peaks.

$$E = \frac{m_4}{m_2^2} - 3$$

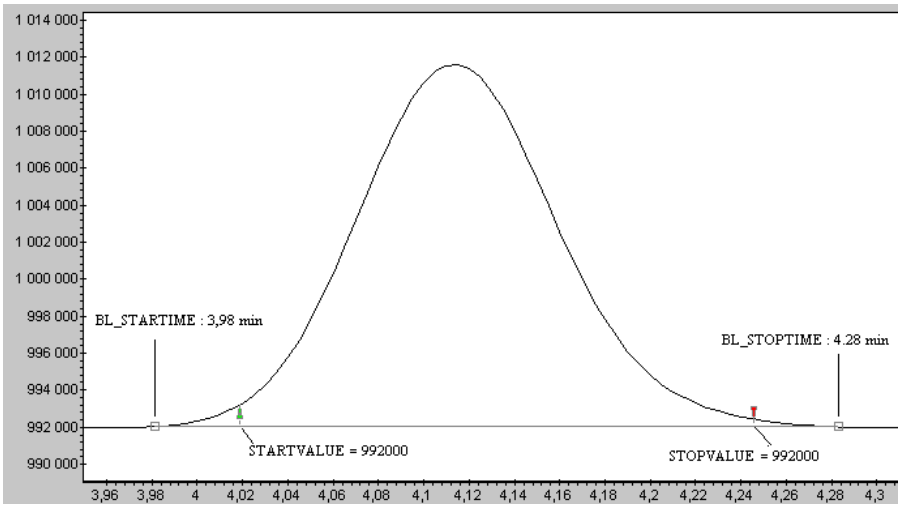
- **Skew [GAMMA]:** γ quantifies the symmetry of a peak.

$$\gamma = \frac{m_3}{m_2^{3/2}}$$

A symmetrical peak has a skew of zero, whereas a peak that tails has a positive skew and a peak that fronts has a negative skew.

Others

- **# Baseline [BASELINEID]:** Peak Baseline Identifier: Index of the peak baseline
- **Baseline Start Time [BL_STARTIME]:** Time of the start marker of the baseline.
- **Baseline Stop Time [BL_STOPTIME]:** Time of the stop marker of the baseline.
- **Baseline Start Value [BL_STARTVALVUE]:** Value of the signal of the baseline at the start peak time.
- **Baseline Stop Value [BL_STOPVALUE]:** Value of the signal of the baseline at the stop peak time.



- **Group(s) [PEAK_GROUP]:** Peak Group(s): The name(s) of the group(s) this peak belongs to.
- **Is Unknown [ISUNKNOWN]:** This variable equals TRUE if the peak is unknown (namely has not been identified) or FALSE if not.
- **Manual RF [ISRFMANUAL]:** This variable is TRUE if the peak has been calibrated in manual mode. Otherwise, it is FALSE.
- **Positive [ISPOS]:** This variable equals TRUE if the peak is a positive peak or FALSE if not.
- **Regression model [REGRMODEL]:** The regression model of the calibration curve used for peak quantification.
- **Response factor_relative standard deviation [RF-RSD]:** Expressed in percent. Obtained by multiplying the RF-SD by 100 and dividing the product by the RF of the associated calibration curve.
- **Response factor_standard deviation [RF-SD]:** Measures the dispersion of the response factors of the different points in the associated calibration curves.
- **Weighting factor [WEIGHTFACTOR]:** The weighting factor applied to the calibration curve used for peak quantification.

Group System Variables

The group variables can be displayed in the group result table. Select ‘report Properties’ in the popup menu of the group result table and select the variables to display. It is possible to save the group report formats as the peak report formats in a library, see page 101).

CompassCDS calculates the following variables for each peak group:

- **Area [µV.min] [G_AREA]** The area is the sum of the areas of all peaks in the group.
- **Area [%] [G_AREAP]:** The area percentage is the area of the group divided by the sum of the areas of all the groups, multiplied by 100.
- **Control sample [G_CTRLSAMPLE]:** Quantity entered in the calibration table for the control sample. This value is used for the control sample computations.
- **Height [µV] [G_HEIGHT]:** The height is the sum of the heights of all peaks in the group.
- **Height [%] [G_HEIGHTP]:** The height percentage is the height of the group divided by the sum of the heights of all the groups, multiplied by 100.
- **Manual RF [G_ISRFMANUAL]:** This variable is TRUE if the group has been calibrated in manual mode. Otherwise, it is FALSE.

- **Name [G_NAME]:** Group Name: Name of the group after identification
- **Number of peaks [G_NBPEAKS]:** The number of peaks included in a group.
- **Quantity** [unit] **[G_QTY]:** The quantity of the group. It equals the sum of the quantity of the group peaks.
- **Qtable** [unit] **[G_QTABLE]:** The Quantity entered in the calibration table for the group and for the corresponding chromatogram level if the chromatogram is a standard or a control sample with level.
- **Recomputed RF [G_RF_Rec]:** It is the recomputed response factor of the group.

For calibration group, if 'curve' factor is used: the response factor is the ratio of the quantity (read in the calibration curve) of the group by its response. If 'manual' factor is used: it is the ratio of the quantity calculated without M, D, mass or Normalization factor, by its response.

For result group, it is the ratio of the quantity calculated without M, D, mass or Normalization factor, by its response.

- **Recomputed RRF [G_RRF_Rec]:** It is the recomputed reverse response factor of the group. It is the reverse of the Recomputed Response Factor of the group.
- **Regression model [G_REGRMODEL]:** The regression model of the calibration curve used for group quantification.
- **Response [G_RESP]:** The response is either the total area, the height, the area% or the height%, the area$^{1/2}$ and the height $^{1/2}$ of the group, according to the choice made in the calibration method.
- **Response factor relative standard deviation [G_RFRSD]:** The response factor relative standard deviation is expressed in percent. It is obtained by multiplying the RF-SD by 100 and dividing the product by the RF of the associated calibration curve.
- **Response factor standard deviation [G_RFSD]:** The response factor standard deviation Measures the dispersion of the response factors of the different points in the associated calibration curve.
- **RF [G_RF]:** This is the response factor of the group. The response factor can be entered in the calibration table if the group is a calibration group, or it is the ratio of the quantity of the group to its response.
- **RRF [G_RRF]:** It is the inverse response factor of a group: RRF = 1/RF= Group response / Group quantity.
- **Weighting factor [G_WEIGHTFACTOR]:** The weighting factor applied to the calibration curve used for group quantification.

Global System Variables

The global variables belong to the whole chromatogram. They can be displayed in the chromatogram properties. Select the menu options DATA / CHROMATOGRAM PROPERTIES in the main menu.

Output Variables

CompassCDS Chromatography Data System automatically computes the following variables for each chromatogram:

- **# id. Peaks [NBIDPEAKS]:** Number of peaks defined in the peak identification tale.
- **Acquisition Method Name [ACQMETHODNAME]:** Name of the method used to acquire the chromatogram.

- **Acquisition Method Version [ACQMETHODVERSION]:** Version of the method used to acquire the chromatogram.
- Acquisition Date & Time [ACQTIME]: Acquisition date and time.
- **Calibration curve [CALNAME]:** The name of the calibration file associated to the chromatogram. If no curve, the value is an empty string.
- **Calibration type [CALTYPE]:** The type of calibration. The variable equals 0 if working in 'Response %', 1 in 'Normalization', 2 in 'External Standard', 3 in 'Internal Standard'.
- **Channel number [CHANNELNUMBER]:** A sample can be acquired on several channels, and a chromatogram is drawn for each channel. This variable gives the channel number of the chromatogram that is selected.
- Chromatogram Name [CHROMATONAME]: The name of the chromatogram.
- **Data path [DATAPATH]:** The data path of the currently connected user. This is the path of the directory containing the files, which is accessible by the current user.
- **Data saved [DATASAVED]:** This variable equals "True" if the chromatogram has been saved or "False if there were changes since the last time the chromatogram was saved. This variable can be used for mapping purposes: if the value of this variable is printed and should equal 'Yes', this will ensure that all the results that are printed are saved, and thus that there is a record of them and the way in which they were obtained.
- **Detector name [DETNAME]:** The name of the detector of the current channel.
- **Drift [DRIFT]:** This variable is the slope (a) of the regression straight line y=ax+b calculated with the "Compute noise On" and Off events (see noise variable).
- **Fraction collection log name [FRACLOGNAME]:** The name of the Log file associated to the chromatogram.
- **Fraction collection unit [FRACUNIT]:** The unit defined for the fraction collection (time, slope, level, etc.).
- **Group Name [GROUPNAME]:** The name of the connection group (defined in the CompassCDS Configuration Manager) on which the user has performed the last chromatogram processing.
- **# Groups [NGROUPS]:** The number of groups defined in the chromatogram.
- **#Int.Std.Peaks [ISTDNB]:** The number of internal standards defined in the method.
- **Injector name [INJECTORNAME]:** The name of the injector used for the acquisition.
- **Last calibration date [CALDATE]:** The last modification date of the calibration curve used to process the chromatogram.
- **Level [LEVEL]:** The calibration level if the chromatogram is a standard or 0 if it is an unknown.
- **Method channel [METHODCHANNEL]:** The name of the channel of the method file used to process the chromatogram.
- **Method name [METHODNAME]:** The name of the last method used to process the chromatogram.
- **Noise [NOISE]:** This variable is calculated between limits defined by a "Compute noise On" event and a 'Compute noise Off' event. Inside these limits a linear regression is calculated for the signal. The result is a y=ax+b equation. This regression straight line is subtracted to the signal and the difference between the min and max value of the 'horizontal' signal is calculated. This is then the noise. This variable can be used for blank chromatograms (no peak) during the whole chromatogram.

- **Noise Sdev [NOISE_SDEV]:** Standard deviation of the chromatogram noise. This variable is calculated over the totality of the chromatogram during the integration phase. This variable has no analytical meaning; it is only used for an internal calculation.
- **Number of missing peaks [NBMISSINGPEAKS]:** The number of missing peaks (i.e., peaks present in the peak identification table but not detected).
- **Number of Peaks [NPEAKS]:** The number of integrated peaks.
- **#Points [NPOINTS]:** The total number of the acquired points in the chromatogram.
- **Operator name [OPERATOR]:** The name of the user that performed the acquisition.
- Processing date [PROCESSDATE]: The last processing date.
- **Project name [PROJECTNAME]:** The name of the project in which the acquisition was performed.
- **Report name [REPORTNAME]:** The file name of the report style used to print the chromatogram.
- **Reprocessing list count [BATCHCOUNT]:** The total number of chromatograms in the reprocessing list, if the current chromatogram was reprocessed inside a reprocessing list. If not, the value of the variable is –1.
- **Reprocessing list name [BATCHNAME]:** The name of the reprocessing list of the chromatogram, if it was processed inside a reprocessing list.
- **Reprocessing list position [BATCHPOS]:** The position of the chromatogram in the reprocessing list, if it was created inside a reprocessing list. If not, the value of the variable is -1.
- **Reason for stop sequence [SEQSTOPREASON]:** The reason why the sequence is stopped. If several suitability tests have failed, only one of them is mentioned. This variable is computed at the end of the processing and should not be used in formulae.
- **RMS noise [RMSNOISE]:** To calculate this variable the y=ax+b equation which is in the noise calculation is used, the regression is also subtracted from the signal and then, for each slice of the 'horizontal' signal:

$$\text{RMS\_Noise} = \sqrt{\frac{\sum_{i=1}^{k} signal^2}{k}}$$

- Where k is the number of points.
- The Noise ON and OFF events have to be defined in the integration part of the method to calculate this variable.
- **Run name [RUNNAME]:** The original name of the chromatogram, entered when preparing the acquisition: prefix + Run ID.
- **Sequence count [SEQCOUNT]:** The total number of chromatograms in the sequence, if the current chromatogram was created inside a sequence. If not, the value of the variable is –1.
- **Sequence name [SEQNAME]:** The name of the sequence of the chromatogram, if it was processed inside a sequence.
- **Sequence position [SEQPOS]:** The position of the chromatogram in the sequence, if it was created inside a sequence. If not, the value of the variable is -1.
- **Software current name [SOFTCURNAME]:** The name of the software which has been used to reprocess the selected chromatogram.
- **Software current version: [SOFTCURVERSION]:** The version of the software which has been used to reprocess the selected chromatogram.

- **Software name [SOFTNAME]:** The name of the software that originally created the selected chromatogram.
- **Software version: [SOFTVERSION]:** The version of the software that originally created the data file.
- **Stop sequence [SEQSTOP]:** This variable equals TRUE if the sequence must be stopped after this chromatogram acquisition (due to a suitability test failure) and FALSE else. This variable is computed at the end of the processing and should not be used in formulae.
- **System name [SYSTEMNAME]:** The name of the system used to acquire the chromatogram.
- **Total peak area [TOTAL_AREA]:** The sum of the areas of all peaks in the chromatogram.
- **Total peak height [TOTAL_HEIGHT]:** The sum of the heights of all peaks in the chromatogram.
- **Total peak response [TOTAL_RESPONSE]:** The sum of the responses of all peaks in the chromatogram. The response is Area, Height, Area % or height%, Area $^{1/2}$ or height$^{1/2}$ according to what has been defined in the calibration method.
- **User name [USERNAME]:** The name of the user that performed the last processing.

Input Variables

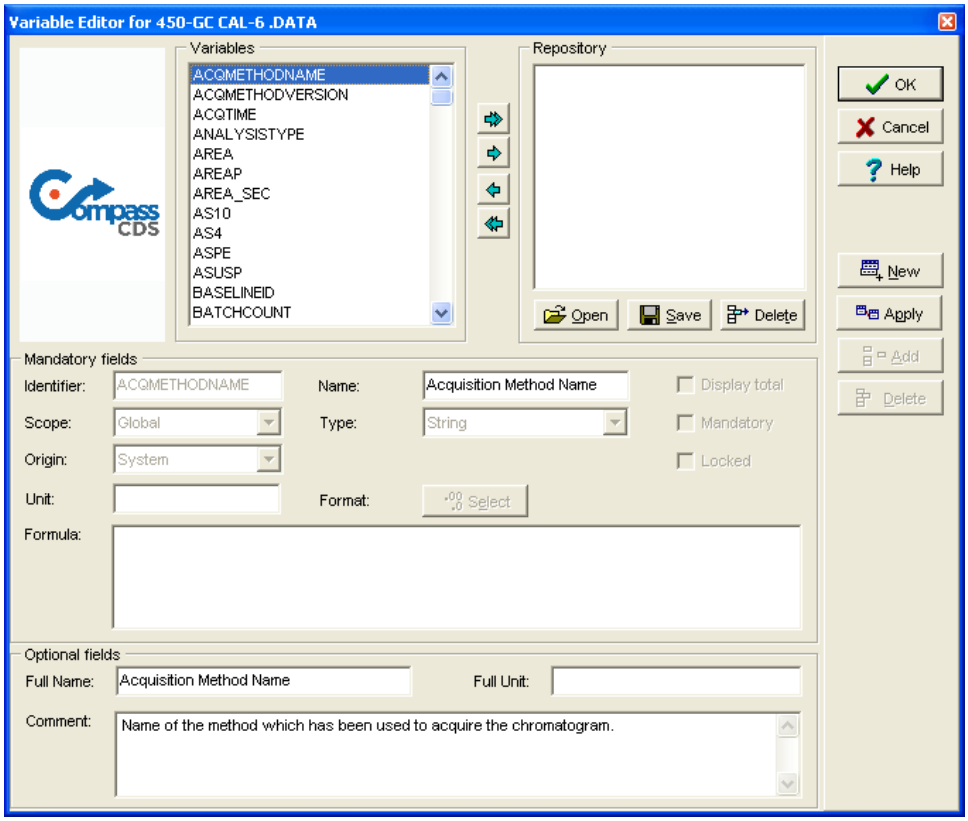
- **Dead time [DEADTIME]:** It is the dead time, entered manually at the acquisition time. It can be modified in the CHROMATOGRAM PROPERTIES after the acquisition.
- **DT [DELTAT]:** The acquisition period. It is the time between two acquisition points. This time can be changed via the Acquisition rate in the acquisition method. Deltat is the inverse of acquisition rate.
- **Divisor Factor [DIVFACTOR]:** This variable is used to divide all the quantities by a factor. This value is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **InjVoL [IVOL]:** This is the volume injected by the autosampler (if present) and if it is driven. It also can be entered for information purposes only. This value is entered when preparing the acquisition. Note that for some liquid chromatographs which injector is chosen, it can be a syringe fraction and not a volume.
- **Istd Weight [ISTDW]:** This is the internal standard quantity, if there is only one. This value is entered when preparing the acquisition and can be modified in CHROMATOGRAM PROPERTIES. When there are several internal standards, use the variable ISTDVAL ('IntStd') that gives the quantity of the internal standard named 'IntStd'.
- **Mass [MASS]:** The mass of injected sample. This value is entered when preparing the acquisition and can be modified in CHROMATOGRAM PROPERTIES.
- **Multiplier Factor [MULTFACTOR]:** This variable is used to multiply all the quantities by a factor. This value is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **#Rack [RACKNUMBER]:** It is the number of the rack used for the acquisition.
- **Run Information [RUNINFO]:** The information about the sample. This information is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **Run Time [RUNTIME]:** It is the total acquisition time of the chromatogram.
- **#Vial [VIALNUMBER]:** The number of the vial where the sample was taken. This value is entered when preparing the acquisition to select the correct autosampler vial (if autosampler is present), or is for information purposes only.

User Input Variables

User input variables are variables created by user who has to assign a value. Two ‘user input’ variables can be defined:

- The ‘user input by peak’ (one value has to be defined by peak)
- The ‘global user input’ (one value has to be defined by chromatogram file)

NOTE: The peak or global choice is made in the “Scope” field.



For both NON MANDATORY ‘global’ and ‘by peak’ user input variables, it is possible to define a default value.

The User Input by Peak Variables

The User-Input variables are variables whose values are entered to be used for the calculation of other variables.

To create a User-Input by peak variable:

1. Add a variable in the variable editor (New button).

   Define the scope: peak.

   Define the origin as “User input”.

   Choose a short, easily remembered identifier for this variable. This identifier can be used in the formula of other custom variables if this variable is needed for other calculations.

   Define the name of the variable. The name will be used to identify the variable in the peak identification table.

Define the unit of the variable. The unit will be associated with the variable name.

Define the type and format of the variable, and optionally, add a comment for this variable.

Check the 'Mandatory' box to require the operator to enter the variable in the identification table (Identification part of the method)

Define a default value for non-mandatory variables only (optional). This option is available only if the user owns the corresponding profile in CompassCDS Configuration Manager.

The 'Lock the variable' function is available only if the user owns the corresponding profile. This option allows the user to lock a variable to forbid other users to modify it, except the format, the unit and the optional fields.

Press the Apply button.

For each peak "user input" variable, a column is added to the peak identification table in which a particular value can be defined for each peak.

Note that if the user modifies the user input default value in a chromatogram, the value is updated in the identification part of the method only for the peak that already contains the previous default value.

Example of "user input by peak" variable: Peak Purity

The analyzed sample can be composed of several compounds coming from solutions of different and known purities. To quantify those compounds, CompassCDS must take into account the purity factor of each peak (if the quantities defined in the calibration table do not take into account the purity).

2. Create a peak user input variable named PEAKPURITY. In the identification table enter the value of the purity for each component in the added column which is the variable name.

   Create a peak user formula with the formula: PEAKPURITY x QTY and display it in the peak result table.

The Global User Input Variables

The global user input variables are variables defined for a chromatogram whose values are entered when starting a single acquisition or a sequence, or in the chromatogram properties. They are entered only for information or to be used for the calculation defined by the user (user formula variable).

- In the Quick Start windows, click on the More button.
- In the sequence, select the "user input" column.
- In the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES select the Variable tab or use the icon).

NOTE: The value entered when starting an acquisition can be changed afterwards, in the chromatogram properties.

To create a new global User-Input variable:

1. Add a variable in the variable editor (New button).
2. Define the scope: global.

3. Define the origin as “User input”.
4. Choose a short, easily remembered identifier for this variable. This identifier can be used in the formula of other custom variables if this variable is needed in other calculations.
5. Define the name of the variable. The name will be used to identify the variable in the acquisition window (Quick Start or sequence) and in the chromatogram properties.
6. Define the unit of the variable. The unit will be associated with the variable name.
7. Define the type and format of the variable, and optionally, add a comment for this variable.
8. Check the ‘Mandatory’ box to require the operator to enter the variable in the chromatogram properties, the Quick start or the sequence.
9. Define a default value for non-mandatory variables only (optional). This option is available only if the user owns the corresponding profile in CompassCDS Configuration Manager.
10. The ‘Lock the variable’ option allows the user to lock a variable to forbid other users to modify it, except the format, the unit and the optional fields. This option is available only if the user owns the corresponding profile.
11. Press the ‘Apply’ button

Note that if user modifies the user input default value in a chromatogram, the value is updated in the chromatogram properties only for the variables that already contain the previous default value.

If loading a chromatogram in a reprocessing list, and then modify the default value of a global user input variable belonging to it, the user will have to load again the method to update the default value. The same behavior occurs in the sequence.

Example of a global user input variable: Sample code

Create a global user input variable called SAMPLECODE. This variable would correspond to a number or a code identifying the analyzed sample. Check the Mandatory Variable box to force the user to assign a value before each acquisition, realized either by a Quick Start or a sequence, in the corresponding field, and press Apply.

User Formula Variables

To create a new variable with specific calculations, press the NEW button. Next, specify the identifier, name and unit of the variable, then specify the scope, to determine if the variable is for the entire chromatogram (global), the groups or the peaks. Finally specify that the origin is a ‘User formula’, complete the corresponding formula (in the Formula field) and press the APPLY button.

How to Express the Formula

The formula definition must follow strict rules:

- The formula can use existing variables. To call an existing variable, use the variable identifier. (For example: AREAP for area percentage or G_RF for the response factor of a group). Enter the first variable identifier letter in the Formula field; a popup menu that lists the variables that begin with that letter is displayed. Choose the variable from the list.
- The mathematical operations of general use (addition, subtraction, multiplication, division) are defined by adding the corresponding symbol (+ - x /), for example: AREA+HEIGHT. More complicated operations are also possible, for example cosine, exponential, logarithm, etc. The corresponding syntax is detailed in the section ‘Usual Functions’, page 134.

- It is possible to define a condition. The correct syntax is:
- If (cond) then (x) else (y) is: IF (cond; x; y). The semicolon means consecutively ‘then’ and ‘else’. Conditions can overlap, so it is important to respect use of parentheses: IF (cond; IF (cond; a;b); IF (cond;x;y)).

For example, if the area of a peak is less than 150, display ‘quantity * 2’, else display “quantity * 3” is: IF (AREA<150; QTY*2; QTY*3).

The results can be real numbers, or strings. The results can also be another condition: IF ((AREA>1000); (IF HEIGHT>1000; ‘Large and high peak’; ‘Large and low peak’); (IF SKEW>=0; ‘Little tailing peak’; ‘Little fronting peak’)). In this case, the area of the peak will first be tested, then if it is larger than 1000, the height will be tested. If the peak area is less than 1000, the skew of the peak will be tested, otherwise the message 'Large and low peak appears'.

- To display text, enclose it with apostrophes; in this way CompassCDS will be able to distinguish it from a variable.
- For example, to create a variable allowing the display of the name on the chromatogram, the retention time and the area of each peak separated by a dash, define a peak variable with the formula: NAME+‘-’+RF+‘-’+ AREA. The result will be, for example, benzene-1,2-34.
- Global, group, and peak variables can be calculated with a user formula. But, if a peak variable is used in a global or a group variable formula, it is necessary to define which peak is addressed. For example if a global formula is the sum of the area of all the peaks divided by the area of the peak of Acetone: the formula will be TOTAL_AREA/AREA(‘Acetone’).The peak name must be defined between apostrophes and parentheses, with exactly the same spelling as the one defined in the identification table.

Of course, it is necessary to clearly define the group used in a global variable formula.

- The groups or the peaks can be defined by their index or by their name. Height (1) will be the height of the first peak, whereas G_QTY (‘NC12+’) will be the quantity of the group named NC12+. The name of a peak or a group is a string character. As a consequence, it is necessary to place it between two single quotes. Peak names are not case sensitive.
- A peak variable without an index or peak name will correspond to the value of the variable for the current peak. For example, the following formula AREA/AREA (‘ISTD’) will divide the area of each peak by the area of the peak named ISTD.
- In the same way, a group variable that is not identified with any index or name will be considered as the variable of the current group in a group variable.
- It is also possible to define a Boolean. A Boolean is composed of a condition expressed as a formula: *Qty (‘Benzene’) <5 or NOISE>100*. The result is True if the condition occurs or False if it is not. The condition can be composed of several conditions separated by AND, OR. Use parentheses to separate the propositions. For example (AREA<5) OR (AREA>30), if one or the other condition is accepted, the result is TRUE if no one is accepted the result is FALSE.
- To set response values other than TRUE and FALSE, use the functionality IF: IF (condition; positive result; negative result). Therefore, if the condition is true, the value of the variable will be the positive result. Otherwise, if it is false, it will be the negative result.

A Few Examples of Custom Variables

- **Annotation (peak variable):** To display the name of the peak and its retention time as the peak annotation, enter the formula NAME+ ‘ ‘ +RT. Once this variable is defined, call it from the Content zone of the peak annotations ( ).

- **Drift:** To calculate the drift between the first and the thousandth data point, the difference between the signal values at these points can be calculated. Create a global variable with the formula DATA (1000)-DATA (1). The result will be displayed in the chromatogram properties.
- Molar response percentage (by peak):

This requires the creation of three variables:

1. A peak user input whose name is MOL_RF. The corresponding values must be entered in the peak identification table for each peak.
2. A peak user formula, whose name can be INTERM, that will be used as an intermediary variable and defined by the formula: AREA *MOL_RF and calculated for each peak.
3. A peak user formula, which is the molar percentage of each peak, defined by the following formula: INTERM/SUM (‘INTERM’)*100. The user will just have to display this variable in the peak result table to know the molar percentage of each peak.

Name of the internal standard associated to each peak:

Three peak user formula variables must be created:

- ISTDINDEX (integer) : ISTD(NAME)
- ISTDNAM (string): NAME(ISTDINDEX)
- ASSOCISTDNAME (string): IF(PEAKID=ISTDINDEX;’ ‘;ISTDNAM)

Display the ASSOCISTDNAME variable in the peak result table. The internal standards will be assigned an empty value; the no internal standard one will be assigned the name of the associated internal standard.

- Name of peaks that are internal standard

In this case only one internal standard is defined; create the following peak user formula:

IF (NAME=ISTDNAME (1);'ISTD';' ')

The value of the variable will be ISTD for the peak that is internal standard and nothing for the non ISTD compounds.

In the case two internal standards are defined, create the following peak user formula:

IF ((NAME=ISTDNAME (1)) OR (NAME=ISTDNAME (2));'ISTD' ;')'

The value of the variable will be ISTD for the peak that are internal standards and nothing for the non ISTD compounds.

- Calculation of the capacity factor according a non fixed dead time value.

Two variables must be defined; one to impose the dead time equal to the retention time of the first integrated peak, the second one to calculate the capacity factor according to the value of the calculated dead time:

1. A global user formula variable, whose name is EXPDEADTIME (experimental dead time) (real) defined by the formula: RT(1)
2. A peak user formula, whose name is CAPACITY(capacity factor) (real) defined by the formula: (RT- EXPDEADTIME)/ EXPDEADTIME

- **Noise:** To calculate the noise between 1 and 2 minutes, the difference between the signal maximum and minimum can be calculated. Create a global variable with the formula 'DATAMAX (1.0; 2.0) - DATAMIN (1.0; 2.0)'. The result will be displayed in the chromatogram properties. Note that the standard system variable Noise_SDEV calculates an estimation of channel noise standard deviation.
- **Relative area (group variable):** To divide the area of each group by the area of the peak named Butadiene, the corresponding formula is 'G_AREA/AREA ('Butadiene')'. Once this variable is defined, it is possible to display it in the group report.
- **Peak validity 1:** To check that the quantity is between 10 and 20 for each peak, create a peak variable with the following formula: IF ((QTY>=10) AND (QTY <=20); 'OK'; 'not OK'). If this variable is selected in the peak report, a new column will appear, stating OK if the quantity of the peak is between 10 and 20 or alternatively not OK if the quantity is not between 10 and 20.
- **Peak validity 2:** There is another way of processing to obtain a similar result. Define a Boolean with the formula (QTY>=10) AND (QTY <=20). The result will be either 'True' or 'False'.
- **Prefix:** To display the RUNNAME without the RUN ID. Create a global user formula, with the following formula: COPY (RUNNAME; 1; POS ('-'; RUNNAME)-1).
- **Relative Response Factor (peak variable):** To divide the response factor of each peak by the response factor of a defined peak, the corresponding formula is 'RF/RF (name of reference peak)'. The first possibility is to type the name of the peak instead of 'name of reference peak' in the formula, the second possibility is to create a global variable (for example 'RefName'), which is a user input and mandatory. The formula should be changed into 'RF/RF (RefName)'. Before acquisition, the user will enter manually the name of the reference (a default value can be entered for the method), and all the response factors of the peaks will be divided by the response factor of the compound whose name will be specified in the acquisition window.
- **Relative Quantity:** To calculate the difference between the quantity of a peak and the quantity of the previous peak, divide it by the height of the next peak. Define a peak variable with the following formula: (QTY-QTY (PEAKID-1))/HEIGHT (PEAKID+1).
- To calculate the area of the 10th peak plus the area of the peak named 'Benzene' and divide the result by the sample weight. Create a global variable with the following formula: (AREA (10) +AREA ('Benzene'))/ SMPWT. The corresponding variable will be displayed in the chromatogram properties.
- How to print only a part of a variable value. For example the name of chromatogram is 'test-1', and you want to print only 'test'. Create a global variable with the following formula: COPY (CHROMATONAME; 1; POS ('-'; CHROMATONAME)-1).

Usual Functions

The list of the usual functions proposed by CompassCDS is detailed in this part of the manual, as the syntax to respect (parenthesis, cots, etc.)

In the following paragraph, X represents the identifier of the variable on which the calculation is performed.

- **ABS(X):** The result of this function is the absolute value of the parameter. For example: ABS (SKEW)).
- **ARCTAN(X):** The result of this function is the arctangent of the parameter.
- **BOOLEAN:** This function transforms the character strings 'TRUE' and 'FALSE' into the Boolean values TRUE and FALSE.

- **CALCOEFF (‘compound name’; ‘coefficient’):** The result of this function is the value of the specified coefficient in the calibration table of the compound defined in the parameters. For example, CALCOEFF (‘Benzene’;’ a') gives the value of the coefficient of the benzene calibration curve.
- **CALCOEFF ('compound name '; ‘COR’):** Using the previous function, enter the special coefficient ‘COR’, and the result will be the regression coefficient of the specified compound curve.

For example, CALCOEFF (‘Benzene’;’ OR')

- **COPY(X; Y; Z):** The result of this function is a part of a variable value. X represents the variable name, Y the position of the first character to copy, Z the position of the last character to copy. For example the chromatogram name is ‘first-quality-test’, and you want to display ‘quality’, the variable to create is: COPY (CHROMATONAME;7;13), where 7 corresponds to the position of the ‘q’ and 13 to the position of the ‘y’ in the entire chromatogram name.
- **COS(X):** The result of this function is the cosine of the parameter.
- **CSUM (‘X’):** The result of this function is a real number, and is the cumulative sum of the variable for the peaks or groups (depends if it is a peak or a group variable). The variable to be summed should be a real number. For example, if the areas of the three peaks of a chromatogram are 10,000; 50,000 and 20,000, then CSUM (‘AREA’) equals 10,000 for the first peak, 60,000 for the second peak, and 80,000 for the last peak.
- **DATA (integer) or DATA (real):** The result of this function is a real number, and is the value of the signal for the slice or the retention time that is given as the parameter. If the parameter is a real, the value of the signal at the corresponding retention time will be given. However, if the parameter is an integer, the value of the signal at the corresponding slice number will be given. Data (10) will be the signal value of the 10th slice, while Data (10.0) will be the signal value at the 10th minute.
- **DATAMAX (integer; integer) or DATAMAX (real; real):** The result of this function is a real number, and is the maximum value of the signal between the two slices (if arguments are integer) or between two times (if arguments are real). The corresponding slices or times are defined as parameters.
- **DATAMIN (integer; integer) or DATAMIN (real; real):** The result of this function is a real number, and is the minimum value of the signal between two slices (if arguments are integer) or between two times (if arguments are real).The corresponding slices or times are defined as parameters. Datamin (0, 1000) will be the minimum value of the signal between the first and the 1000th slices. Datamin (8.2, 8.5) will be the minimum value of the signal between 8.2 and 8.5 min.
- **Date:** This function provides the current date. The result of this function is a string. For example, the value of this function could be ‘10/07/99’.
- **DAYSBETWEEN:** This function is useful to calculate the number of days between two dates. DAYSBETWEEN (a; b) compares the number of days between a and b. The result is an integer. For example
- DAYSBETWEEN ('01/12/99'; ACQTIME),
- DAYSBETWEEN ('today'; CALDATE),
- DAYSBETWEEN ('December 12, 1999';'january 1, 1998'),
- DAYSBETWEEN ('today';'monday').
- The character strings describing the dates will follow the regional settings for Windows.
- **EXP(X):** The result of this function is the exponential of the parameter.

- **FLOAT(X):** This function is the inverse of string: it transforms the parameter (integer or Boolean) into a real number if possible. In the case of a Boolean value, TRUE is transformed into 1.00 and FALSE is transformed into 0.00.
- **FRAC(X):** The result of this function is the decimal part of the parameter. For example, FRAC (11.258) is 0.258.
- **GROUPID:** This function is useful for group variables. It provides the index of the group for which the variable value is calculated. For example, AREA (GROUPID)/AREA (GROUPID-1) will be used to calculate the ratio of the area of the current group to the area of the previous group.
- **INT(X):** The result of this function is the whole number part of the parameter. For example, INT(11.258) is 11.0. The result is a real number, whereas the result of TRUNC is an integer.
- **ISTD ('compound name') or ISTD (NAME):** The result of this function is the index of the internal standard associated with the peak or the group set as a parameter. If a peak variable is created with the formula 'ISTD (NAME)', the index of the internal standard associated with each peak in the peak table will be displayed.
- **ISTDNAME (I):** The result of this function is the name of the ith internal standard (in the order of appearance in the chromatogram properties).
- **ISTDVAL ('IntStd'):** The result of this function is the quantity entered for the internal standard which name is 'IntStd'.
- **LENGTH(X) or LENGTH ('text'):** This function gives the number of characters in the string set as a parameter. For example, LENGTH ('STRING')=6.
- **LN(X):** The result of this function is the natural logarithm of the parameter.
- **LOWER(X) or LOWER ('text'):** This function transforms the character strings into lower case. For example, LOWER ('STRING') ='string'.
- **MAX ('X') or MAX ('X'; n):** This function calculates the maximum value of the peak or group variable defined as a parameter. This function can also be used to calculate the nth maximum value. For example, MAX ('HEIGHT';2) is the second maximum height.
- **MAXID ('X') or MAXID ('X'; n):** This function calculates the index of the peak (or group) which has the maximum value for the variable defined as a parameter. This function can also be used to calculate the index of the peak or group that has the nth maximum value.
- **MIN ('X') or MIN ('X'; n)::** This function calculates the minimum value of the peak or group variable defined as a parameter: MIN('AREA') is the minimum area of the peaks. This function can also be used to calculate the nth minimum value: MIN ('G_AREA'; 2) is the 2nd smallest group area.
- **MINID ('X') or MINID ('X'; n)::** This function calculates the index of the peak (or group) which has the minimum value for the variable defined as a parameter: MINID('AREA') is the index of the smallest peak. This function can also be used to calculate the index of the nth minimum value: MINID ('G_AREA'; 2) is the index of the 2nd smallest peak.
- **PEAKID:** This function is useful for peak variables. It provides the index of the peak for which the variable value is calculated. For example, AREA (PEAKID)/AREA (PEAKID-1) will be used to calculate the ratio of the area of the current peak to the area of the previous peak.
- **PI:** is the constant π.
- **POS(X;Y):** This function gives the position of a character (or a group of characters) in a variable. For example you want to know the position of 'quality' in the chromatogram name 'first-quality-test'. The variable to create is POS ('quality'; CHROMATONAME), the result is 7, corresponding to the position of the q in the chromatogram name.

- **POWER (a; b):** This is a two-parameter function: POWER (a; b) is equal to “a” to the power of “b”.
- **REALEQUAL (a; b; c):** This function is used to compare two real numbers. The result of REALEQUAL (a; b; epsilon) is TRUE if “a” equals “b” within the tolerance epsilon, e.g. REALEQUAL (HEIGHT; 10,000; 10) will be true if the height is between 9,990 and 10,010.
- **ROUND(X):** This function is used to transform a real number into an integer by rounding it to the closest integer. ROUND (11.8) is 12 and ROUND (11.49) is 11.
- **SIN(X):** The result of this function is the sine of the parameter.
- **SQR(X):** The result of this function is the square of the parameter.
- **SQRT(X):** The result of this function is the square root of the parameter.
- **STRING(X):** This function transforms the parameter (a real number) into a character string: STRING (1.23) is ‘1.23’.
- **SUM (‘X’):** The result of this function is a real number and is the sum of the variable for all the peaks or groups (depending if it is a peak or a group variable). The variables to be summed should be real numbers. For example, SUM (‘AREA’) equals the variable TOTAL_AREA and is the sum of the areas of all the chromatogram peaks.
- **Time:** This function provides the current time. The result of this function is a string. For example, the value of this function could be ‘15:22:30’.
- **TRUNC(X):** This function is used to transform a real number into an integer by deleting the decimal part of the number. Example: TRUNC (11.8) is 11.
- **UPPER(X) or UPPER (‘text’):** This function transforms the character strings into upper case. For example, UPPER (‘String’) =’STRING’.
- **+:** This function is useful to attach several character strings: ‘Date: ’+Date equals ‘Date: 6/16/99’. The result of an attachment with a character string will always be a character string.

Variable Repository

The variables are associated with a method. If a variable is defined in a method, and is needed for use in another method, the variable can be stored in the repository:

Define the variables needed in the first method.

In the variable editor, click and drag them to the repository, or move them with the arrows (and). It is possible to remove some variables from the repository using the Delete button.

Save the repository using the Save button.

In the other method, open the repository using the Open button.

Import the variables needed using the button.

It is possible to use the repository to move the changes that were made on the standard variables (name, format…). Save the corresponding variables in the repository, open it in the method, and then import them as different variables.

A repository named ‘Additional variables.REPO’ is available. It contains the following peak variables.

AS13: peak asymmetry (half width at 13,4%).

AS32: peak asymmetry (half width at 32,4%).

AS50: peak asymmetry (half width at 50%).

AS60: peak asymmetry (half width at 60.7%).

FLAG1: If the peak is saturated (value of the ISSAT variable = TRUE), then the variable has the value ‘Saturated’.

FLAG2: If the height of the peak is inferior to the value of the LOQ variable (limit of quantification), then the variable has the value ‘Below LOQ’. Do not forget to add the LOQ variable in the variable list.

FLAG3: If the start or stop peak markers have been defined manually, the variable has the value ‘Manual integration’.

FLAG4: If the height of the peak is inferior to the value of the LOD variable (limit of detection), then the variable has the value ‘Below LOD). Do not forget to add the LOD variable in the variable list.

LOD: Limit of detection, the variable equals to NOISE*3 (do not forget to add the COMPUTE NOISE ON and OFF integration events in the integration table).

LOQ: Limit of quantification, the variable equals to NOISE*5 (do not forget do add the COMPUTE NOISE ON and OFF integration events in the integration table).

PEAK SIGN: If the ISPOS variable value is ‘TRUE’, ‘the variable has the value ‘positive’ and ‘negative’ if not.

P_ANNOTATION: If the peak is identified, the variable value is the name of the peak. If it is an unknown the variable value is its retention time.

P_ANNO_NAME_QTY: The variable value is the name of the peak plus its quantity plus its unit. Do not forget to edit the variable and replace the word ‘unit’ by the correct unit in the formula field.

P_ANNO_NAME_RF: The variable value is the name of the peak plus its response factor.

P_ANNO_NAME_RT: The variable value is the name of the peak plus its retention time.

P_ANNO_RT_NAME: The variable value is the retention time of the peak plus its name.

P_ANNO_RT_NAME_AREAP: The variable value is the retention time of the peak plus its name plus its area percent.

P_ANNO_RT_NAME_CODE: The variable value is the retention time of the peak plus its name plus its code (see the CODE variable definition).

P_ANNO_RT_PGROUP: The variable value is the retention time of the peak plus the name of the group it belongs to, if any.

The ‘Additional variables REPO’ file is stored in the COMPASSCDS / SERVER / DATA SHARED directory.

RF_SEC: The variable value is the response factor expressed in Qty unit/µV.sec. It corresponds to the calculation RF*60.

NOTE: For all the annotation variables, do not forget to check the ‘annotate unknown peaks’ option in the peak annotation screen and to select the P_ANNOTATION variable in the Content field.

Baseline Monitoring / Quick Start / Sequence

The baseline monitoring allows the signal generated by the system to be viewed, without the need of any injection. Quick Start and Sequence allows injection of one or several samples. During a baseline monitoring, no data file is generated whereas during an acquisition (Quick Start or sequence) data files are generated.

Before starting a baseline monitoring or an acquisition, a method must be prepared for the corresponding system (chromatograph).

Baseline Monitoring

To monitor the baseline before starting an acquisition, select the menu ACQUISITION / MONITORING BASELINE.

A window appears in which it is possible to select which system should be monitored. (When logged in with the 'All projects' mode, the project must first be selected). Now choose the method to be used to condition the apparatus: the initial parameters of the method are sent to the system so that it is prepared for the analysis.

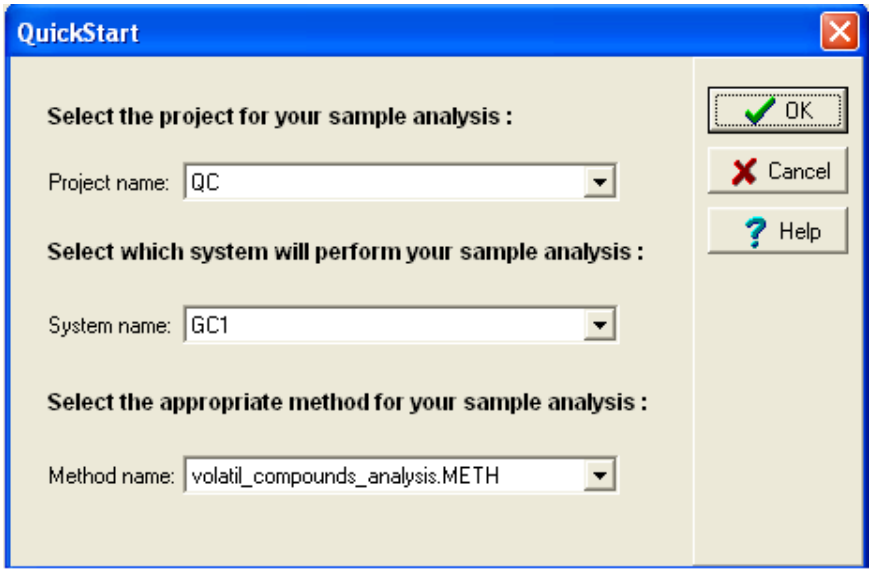
The signal is then displayed in the acquisition window (system tab) as for normal acquisitions. When the system is ready, press the 'stop' button to cancel monitoring and allow the start of an acquisition.

Quick Start

Single Acquisition

To start a single acquisition, select the menu ACQUISITION / QUICK START or press the corresponding icon .

The following window appears:



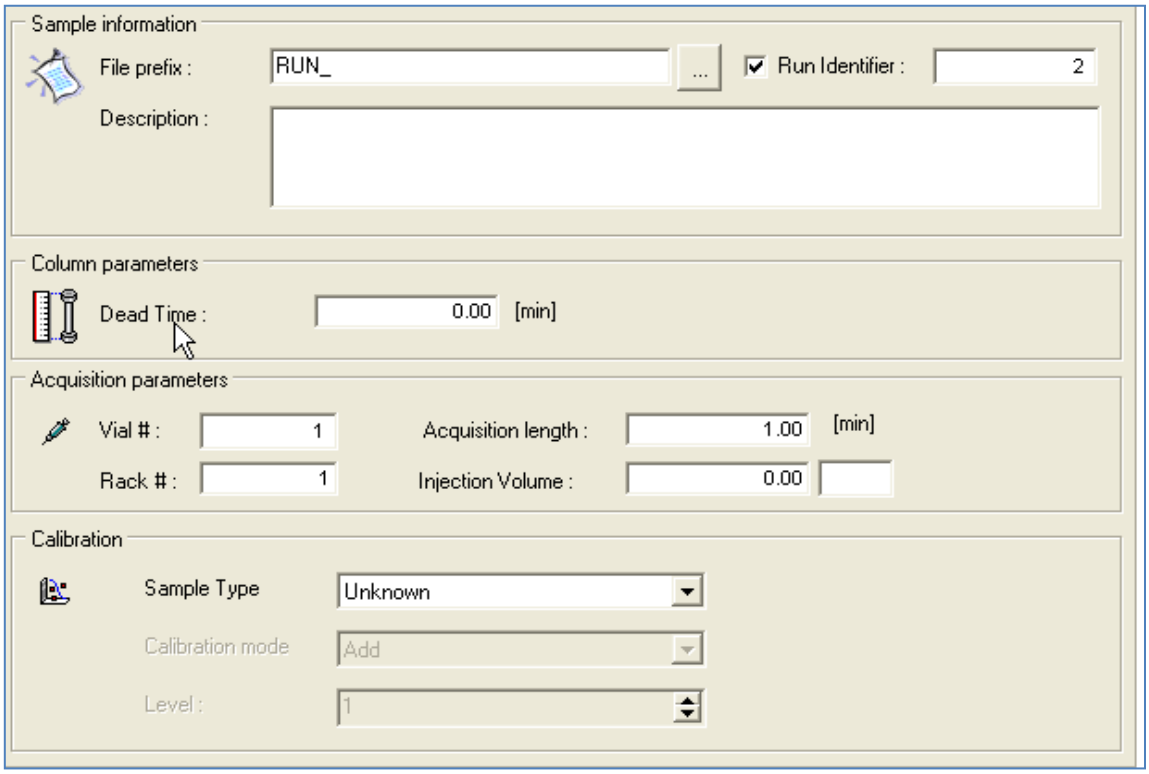
In this window, select the project associated with the acquisition (if connected in all projects). The chromatogram will be stored with the files associated with this project.

Next, select the system (chromatograph) for sample injection. CompassCDS will only display the system names that are associated with the specified project.

Now select the method that will be used to acquire and process the sample. CompassCDS will only display the method names that are associated with the specified system.

Press OK.

The Quick Start window now appears. The default acquisition parameters set in the method are displayed in this window.



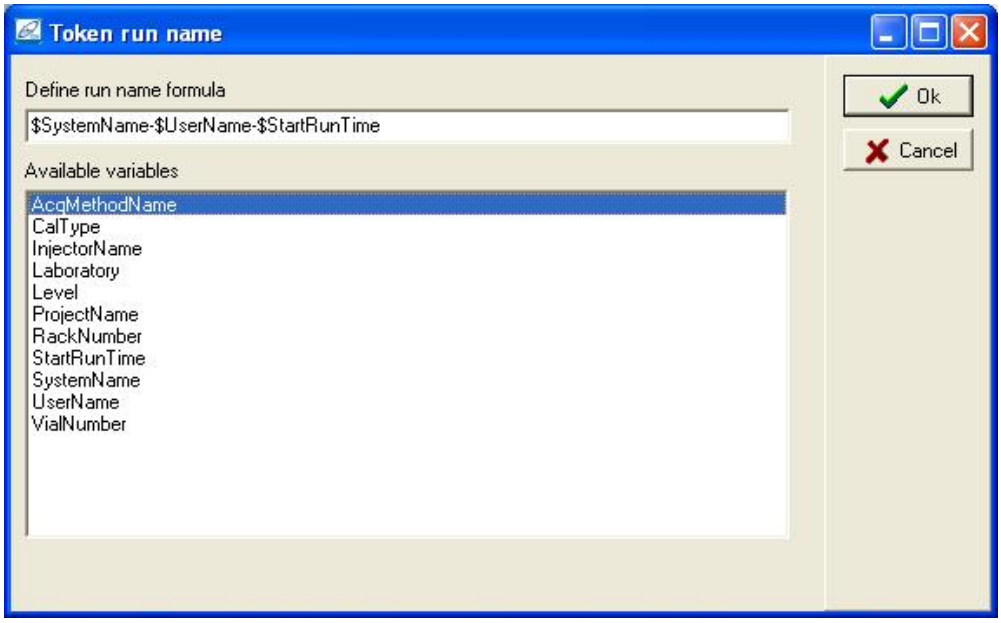
In the Acquisition parameters tab, define all the parameters common to all channels.

The name of the project, system and method just selected are automatically displayed at the top of the window.

In the sample information section, enter:

File prefix: This specified the first part of the chromatogram name. The chromatogram name will be completed with the identifier. The prefix should not contain \ /:*?"<>|.

The prefix can be generated automatically by the software according to variables values. To define the ‘Token run name’, click on the ... button, and compose the token by selecting the variables (double click) in the list:



Run identifier: The second part of the chromatogram name is specified here. The index is automatically incremented in the case of the Quick start.

For example, if the file prefix is 'Run_', and the identifier is 55, the name of the chromatogram will be Run_55.data.

It is also possible to deactivate the Run identifier addition, by unchecking the associated combo box.

NOTE: If the user is not assigned the permission to overwrite chromatogram, and that a chromatogram with the same name as the one defined in the Quick Start screen already exists in the logon path, no message will appear to inform the user, and the generated chromatogram name will be the user defined name plus the acquisition date and time. The existing chromatogram will not be overwritten.

If the user is assigned the permission to overwrite chromatograms, no message will inform him that a chromatogram with same name exists, the chromatogram will be overwritten.

Description: User can enter a description that may be printed in the report.

In the column parameters section, enter the dead time (min)

In the acquisition parameters section, enter:

The vial number (alpha numeric value can be entered according to the sampler type).

The Rack number.

The Injection volume.

The Run Time (total length of the acquisition).

In the Calibration section, enter:

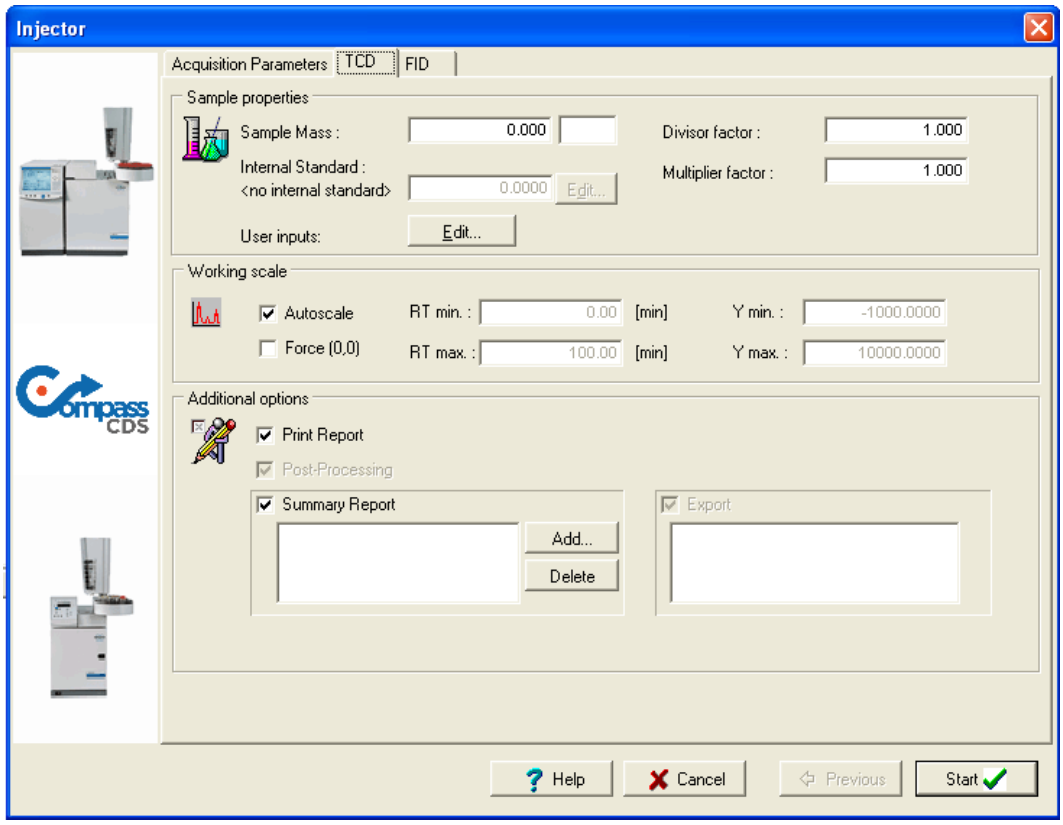
Sample Type: Define whether the chromatogram is a blank, an unknown, a standard, a control sample or a control sample (level I). According to the option selected, the chromatogram process is different.

Calibration mode: This option is available if the user is assigned the right to overwrite calibration curve. It allows the user to delete the existing curve and to build a new one by selecting 'Clear old points', or erase only the points of the defined level by selecting 'Clear level only', or add the calibration point to an existing curve by selecting 'Add'.

Level: This option allows the user to define the level in case of 'Standard or Control Sample (level I) sample' type selection.

NOTE: If the sample type is 'Control sample (level I)', and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level I) in case of suitability test failure.

Select the Channel X tab, to enter the parameters channel by channel. The following screen is displayed:



If a multi channel system is used, CompassCDS offers the possibility to define identical values for all channels (by default) or to enter channel specific parameters if the corresponding option is defined in the chosen method (refer to the 'Acquisition' part of 'The Method' section, page 34). If this option is not defined, the user defines the sample properties and the Working scale only in one tab; the other channel tabs are automatically duplicated.

In the sample properties section, enter:

Sample Mass: The mass of the injected sample

Istd: Internal standard quantity(ies), if defined in the calibration part of the method.

M: Multiplier factor

D: Divisor factor

Global User Input: global variables defined by user.

In the **Working scale** section:

Auto scale: If this option is checked, CompassCDS adjusts the chromatogram Y scale according to the max height signal. If not checked, the user specifies the X and Y limits in the corresponding fields. These limits will be the full scale in the acquisition view (System tab) and in CompassCDS main screen (Data tab) when opening the chromatogram. It is possible to modify the scale of the chromatogram after its acquisition, by pressing the icon (see page 181).

NOTE: If only the part of the signal corresponding to the working scale is displayed on the screen, remember that all points of the chromatogram are stored in the data file and potentially displayable.

Force (0, 0): Forces the acquisition view to display the origin point. This function does not force the signal to pass through the origin.

In the **Processing options** section, specify which parts of the process have to be executed by checking them.

When all the parameters have been defined, press the start button

. The control parameters are transmitted to the system and the acquisition starts immediately or when the CompassCDS Chromatography Data System receives the automatic or manual start.

Note that the ‘Quick Start’ screen is almost the same as the acquisition part of the method one. The format (number of significant digit, scientific format) of some options of the ‘Quick Start’ is customizable in the acquisition screen of the associated method, but NOT modifiable from the ‘Quick Start’ screen. The customized variable formats are:

In the ‘Sample Properties’ part: every variable

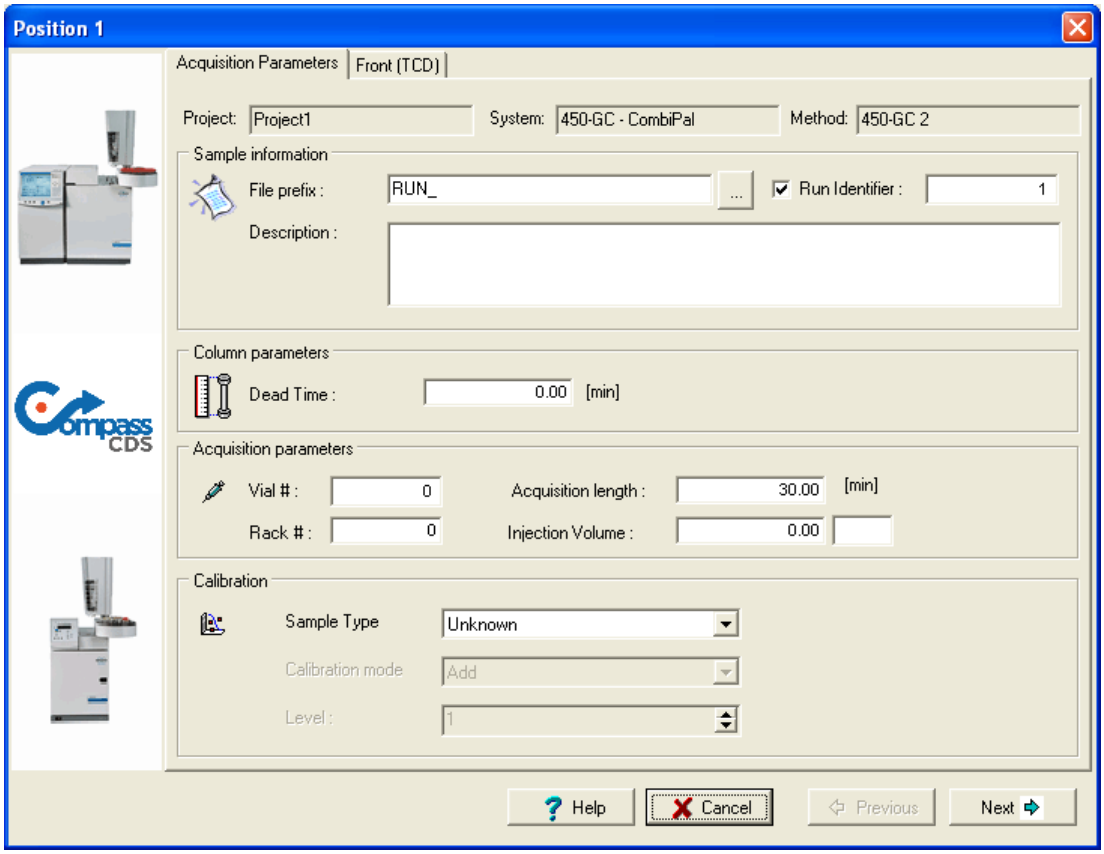
In the ‘Column parameters’ part: the Dead time

In the ‘Acquisition parameters’ part: the Run time

In the ‘Working scale’ part: RT min and RT max

In the case of multi injector systems, the Quick Start function starts as many acquisitions as injectors. As several chromatograms are created (one for each injector), several acquisition windows are completed. Each injector gives its name to the corresponding acquisition window.

Once project, system and method have been selected, the following screen is displayed:

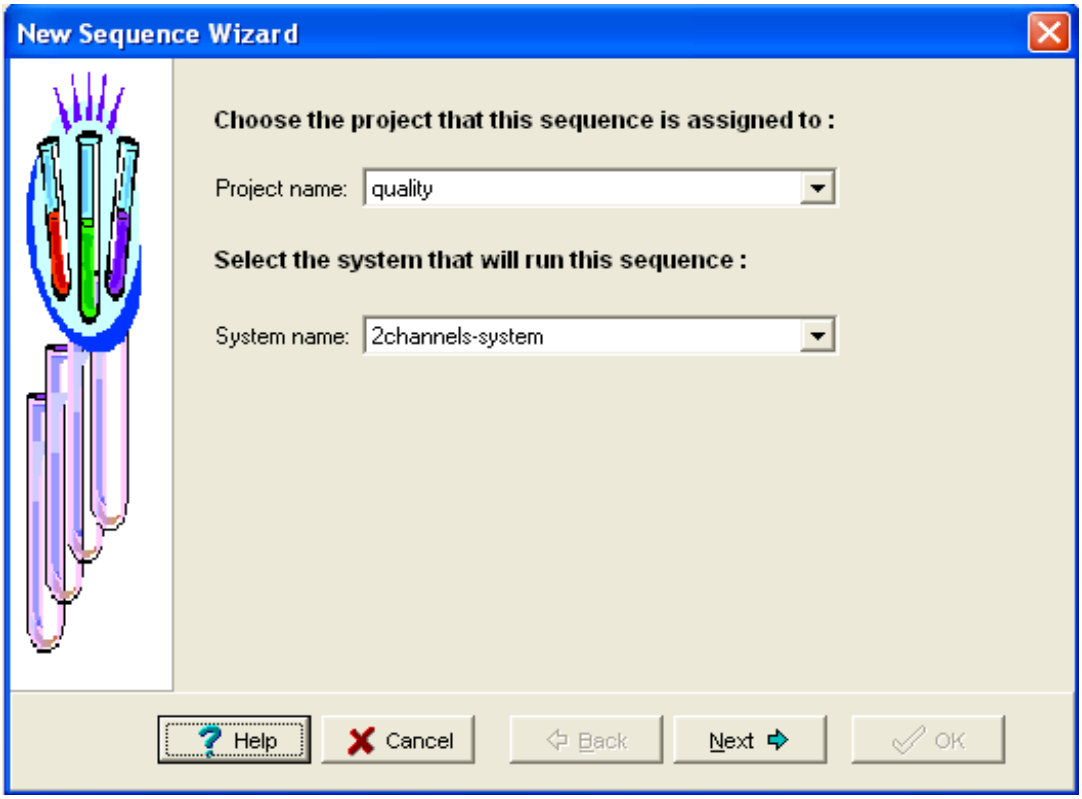


In the first injector acquisition window, the ‘Next’ button allows the access to the second injector parameters, and so on, according to the injector number defined. To come back to the previous injector screens, click on the ‘previous’ button. Once all screens are configured, click onto the ‘Start’ button to launch all acquisitions.

Sequence

To create a sequence: Select the menu options FILE / NEW / NEW SEQUENCE**.**

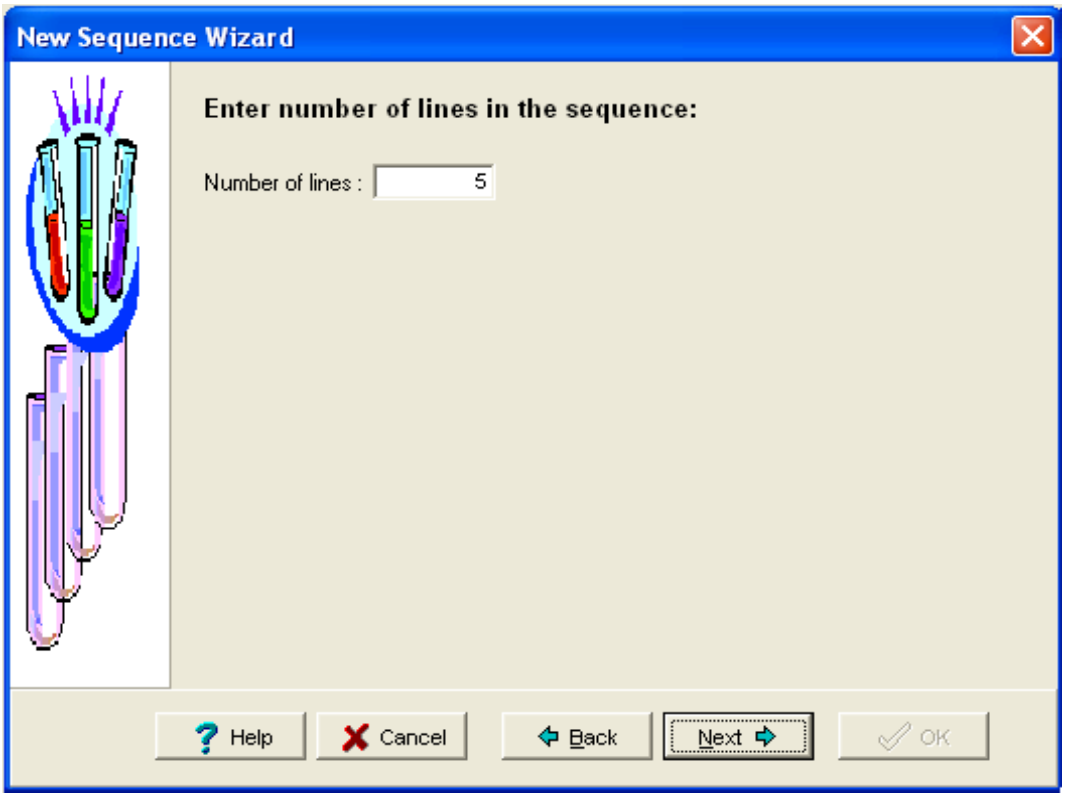
A wizard guide is available for the first steps of the sequence creation:



In this window, select the project associated with the acquisitions (if connected in all projects). The chromatograms will be stored with the files associated with this project.

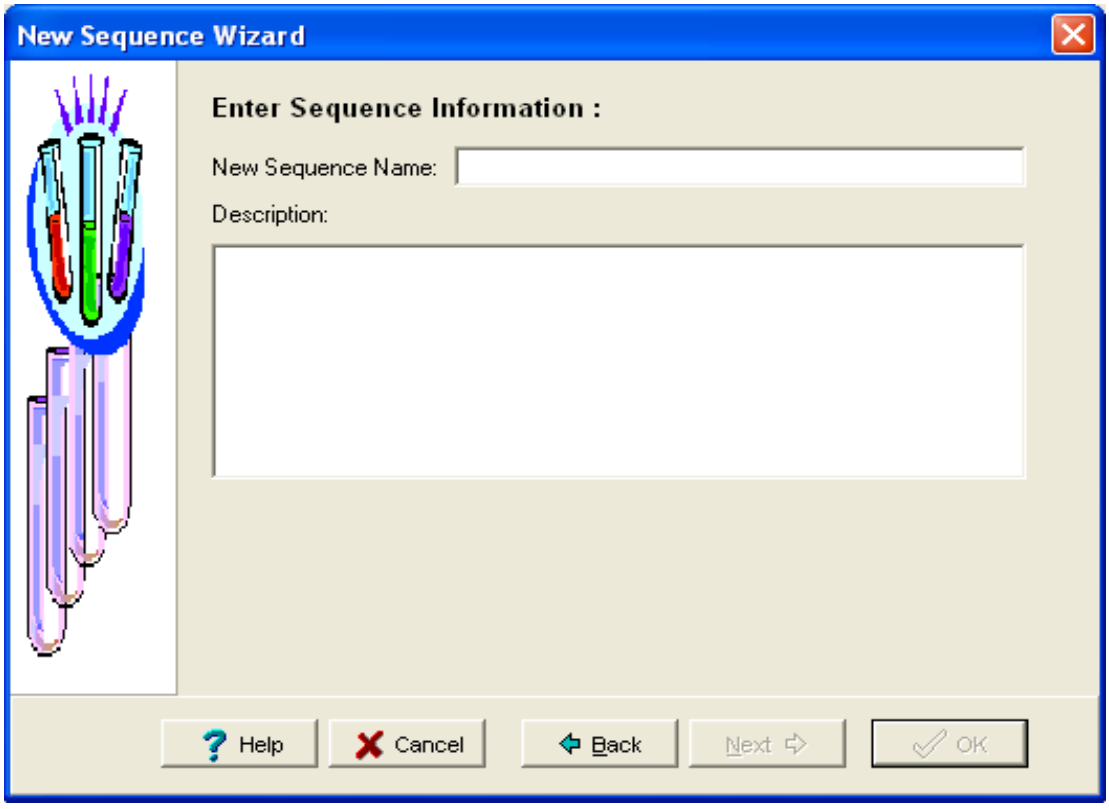
Next, select the system for sample injection. CompassCDS will only display the system names associated with the specified project.

The Next button is now active, and the second step of the method creation can be accessed to specify the number of lines in the sequence:



Each line corresponds to a sample. It is possible to add or delete sequence lines after sequence creation.

Press the NEXT button to access the third step of the sequence creation:



Enter the name of the sequence in the first edit box. In the description field, enter information about the sequence. This information will be displayed in the open file window.

The OK button is now active, after this button is pressed; the sequence is created and opened in CompassCDS.

The following sequence information is displayed at the top of the sequence graphic window:

- The name of the sequence.
- The name of the user connected / the name of the user group / the name of the project containing the sequence / the name of the system associated with the sequence.
- Near this information, the following sequence status information is also provided:

IDLE: This means that the sequence has not been launched yet or is still being created.

BEFORE RUN means that some control parameters have been sent to the system, which is about to start.

RUNNING means that a chromatogram is being acquired.

COMPLETED means that the sequence has been performed without any recorded errors.

ERROR means that a problem has occurred during acquisition. A detailed message will identify which type of error was recorded.

PAUSE AT THE END OF RUN: The sequence has been paused at the user's request, and the acquisition is still running. The user will decide at the end of the run to perform or not the rest of the sequence.

STOPPING RUN: The run is being stopped.

STOPPED: This message means that the sequence has been stopped manually.

PAUSED: This message means that the sequence has been paused manually.

SEQUENCE RESET: This message means that the sequence has been reset and can be re-launched.

CONNECTION LOST: This means that the connection has been lost. This is an abnormal state.

CONNECTION RECOVERED: This means that the connection has been lost and then recovered. No acquisition points should be lost with this type of error.

The Sequence Columns

- **No:** This is the sequence line.
- **Enabled:** This specifies whether the corresponding sequence line acquisition must be performed or not. The acquisition is performed if the box is checked.
- **Method:** In this column the name of the method to be used to acquire and process the chromatogram must be defined.
- **Method properties:** In this column it is possible to deactivate certain process of the chromatogram. Press the button and uncheck any process, which should not be executed at the end of the acquisition (e.g. export, printing, summary report or post processing).

- **Run name (prefix):** Specify the first part of the chromatogram name in this field. The chromatogram name will be completed with the identifier. This part of the name should not contain such characters as \ /:*?"<>|.
- The prefix can be generated automatically by the software according to variables values. To define the 'Token run name', click on the button, and compose the token by selecting the desired variables in the displayed screen. (See Quick Start / Single Acquisition chapter).
- **Run ID (Suffix):** Specify the second part of the chromatogram name in this field. For example, if the file prefix is 'Run_' and the identifier is 55, the name of the chromatogram will be Run_55.data. This parameter has to be an integer.
- **Description:** Information about the run may be entered in this area. This information will be saved with the chromatogram and displayed in the open file window and in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES). The description has a maximum length of 255 characters.
- **Run time:** Specify the total acquisition time in this field. The time should be greater than 0.1 and less than 1000 minutes. The sum of all the run times is displayed at the top of the sequence.
- **Injection Number:** Allows repeat injection of the same sample. The corresponding DATA files suffix will be incremented automatically: e.g. sample1_1, sample1_2.
- **Vial:** The vial number can be entered for information purposes only, or is used to specify which autosampler vial number should be injected if the instrument is controlled. According to the injector installed, alphanumeric values can be entered (refer to the injector constructor manual).
- **Rack:** The rack number is used to specify the rack number, which contains the vial with the sample to be injected if the controlled autosampler contains several racks.
- **Inj. Vol.:** The injection volume can be entered in this cell for information purposes only or can be used to specify injection volume for an autosampler, which is fully controlled by the CompassCDS Chromatography Data System.
- **Sample type:** Define, using this box, whether the injected sample is a standard, an unknown, a blank, a control sample or a control sample (level-I).
- **Calibration:** If the injected sample is a standard, choose whether the calibration point must be added to an existing calibration curve (add), or if the existing calibration curve must be overwritten (clear old points).The last possibility is to delete all the points of the defined level by choosing Clear level only.

NOTE: If the user is not assigned the right to overwrite chromatogram, and that chromatogram(s) with the same name as the one(s) defined in the sequence already exists in the logon path, no message will appear to inform the user, and the generated chromatogram name will be the user defined name plus the acquisition date and time. The existing chromatogram will not be overwritten.

In the other hand, if the user is assigned the right to overwrite chromatograms, no message will inform him that a chromatogram with same name exists, the chromatogram will be overwritten.

NOTE: If the sample type is 'Control sample (level I)', and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level I) in case of suitability test failure.

- **Level:** If the injected sample is a standard or a control sample (level-I), choose the corresponding level in this cell.
- **Istd values:** Press the button to enter the quantity (ies) of the internal standard(s).

- **User input:** In this column, it is possible to specify user input variables if some have been specified in the method.
- **Divisor:** This variable is used to divide all the quantities calculated for unknown samples by a factor. If owning the corresponding profile (to define in CompassCDS Configuration Manager) the quantity of standards will also be divided by this factor.
- **Multiplier:** This variable is used to multiply all the quantities calculated for unknown samples by a factor. If owning the corresponding profile (to define in CompassCDS Configuration Manager) the quantity of standards will also be multiplied by this factor.
- **Sample mass:** Enter the total mass of the sample in this field. This value is mandatory if the calibration mode defined in the method is mass ratio or mass%.
- **Dead time:** This time corresponds to the time required for the sample solvent (or any non-retained compound) to reach the detector. This time is used for the calculation of the selectivity and capacity factor.

NOTE: All the parameters entered in the sequence are saved with the chromatogram. Many are visible in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES) once the chromatogram has been acquired and opened in CompassCDS. The following ones can be modified in the chromatogram properties: user input variables, description, sample mass, divisor, multiplier, dead time, Internal standard values.

Use the icon to hide columns if you do not need to modify their content.

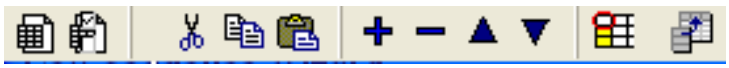
NOTE: If defining “Blank” sample(s) in the sample type column, and using a method with a chromatogram name defined in the pre-processing part, the blank subtracted will be the one defined in the type column.

Filling the Sequence

Each line corresponds to one sample.

In the first column of the sequence, select the name of the method to be used to acquire and process the chromatogram corresponding to the current line. Most of the cells in the line are filled using the values set in the acquisition part of the method, of course, these values can be modified later.

Next, fill the other columns. The sequence bar provides support tools (Most interesting is the Fill block icon):



	This icon clears the content of all the cells of the sequence.
	This icon clears the unchecked lines of the sequence.
	This icon adds a line at the end of the sequence.
	This icon deletes the selected line.
	This icon moves the selected line up.
	This icon moves the selected line down.

	This icon fills several cells of the same column according to the content of the first one. For example, to fill the 'Run ID' column, select the cells to be filled in the column, then fill the first cell with 1. Press this icon. A window appears to define the way the number will be increased. Press *OK*, and the cells are filled. If the column contains a real value or the method, the content of the first cell is simply copied, then pasted in all others.
	This icon permits selected columns to be hidden. Press this icon, and a 'Columns' window appears. Unselect the columns to hide then click on OK. Be careful not to hide cells that must be filled in before the run.

The Method properties, User input, Information and Istd values columns are filled using the button. The size of the columns can be easily modified. Place the mouse between the headers of two columns: the cursor's appearance is modified () then click on the limit between the two columns and drag it to the new position. In the same way, if you click on a column header and drag it to a new position, the column order is modified.

The sequence column order, the size of the columns and the hidden column configurations are saved with the sequence.

Some columns of the sequence have to be filled completely before the sequence is started: the method, Run name, Run ID, Run length, any mandatory user input variables if existing, the internal standards values and sample mass (if working in the corresponding calibration mode).

Once the sequence is filled, save it.

Multi Injector System

CompassCDS can acquire data on multi injector system. The sequence functioning is described below for a double injector.

If a system is composed of two injectors, the sequence works differently. In fact, two acquisitions are run simultaneously on one system. The sequence takes into account the two injectors.

Creation: During sequence creation, the user is asked to enter the number of lines. In the case of double injector, each injector will have the specified number of lines. The total number of lines of the sequence will be two times the specified one. For example, if a sequence is created with 7 lines, the first injector will be assigned 7 lines, the second injector 7 lines, and the whole sequence will have 14 lines.

Method column is not filled in as a single injector sequence. Both lines of the same run must be assigned with the same method. If the method field is entered for the first injector, the second injector one will be automatically copied.

Injector2 | Injector1 | ALL

Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections
1	☑	test.METH	inj2-	1	30	1
2	☑	test.METH	inj2-	2	30	1
3	☑	test.METH	inj2-	3	30	1
4	☑	test.METH	inj2-	4	30	1
5	☑	test.METH	inj2-	5	30	1

Sequence visualization: Three buttons change sequence displaying.

Injector1 Display only the first injector lines.

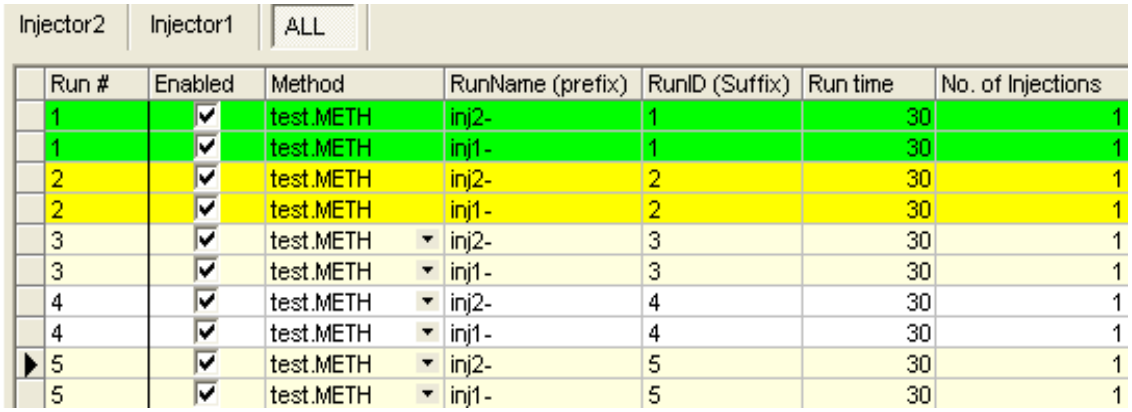
Injector2 Display only the second injector lines.

ALL Display all the lines of the sequence.

Number of lines: Respectively, the + and + buttons add or delete one run (Two lines). Each line corresponds to an injector.

Lines selection: If the two injectors have been selected in the method, every 'Enabled' boxes are active; they can be checked or unchecked according to user need. But if an injector has been unchecked in the method, the corresponding lines will be disabled and inactive in the sequence.

Acquisition: The Start ▶ Pause ❚❚ and Stop ■ buttons work simultaneously for both injectors. The two lines of the same run are acquired at the same time and are displayed in yellow when sequence is running.



If working in Specific Channel Parameters mode, (see acquisition part of the Method section), some variables (Multiplier and Divisor factors, sample mass, Istd values, and User inputs variables) are channel dependent. Meaning that for those variables a value must be entered for each channel (of each injector in the case of a multi injector system).

Some rules have to be taken into account to fill the sequence:

- Fill block for M, D Sample mass: It is best to fill the block from each injector screen, if entered from the ‘All’ screen the value of the first line will be copied on all channels of all injectors.
- Fill block for Istd and User inputs is realized by injector, the values entered for the first injector cannot be copied for the second injector.

Bracketing

With the normal calibration building mode, the standard chromatograms have to be acquired before the unknown ones. However, an option allows you to bracket the unknown chromatograms with standard runs:

To activate the bracketing option, open the sequence and check the ‘Bracketing’ box, in the top right part of the sequence. The Calibration column disappears and a Bracketing column appears.

To bracket samples by certain standards, fill the sequence in the acquisition order and enter the same bracketing identification, B1 for example, the following acquisitions can then be part of another bracketing.

Two bracketing can be overlaid:

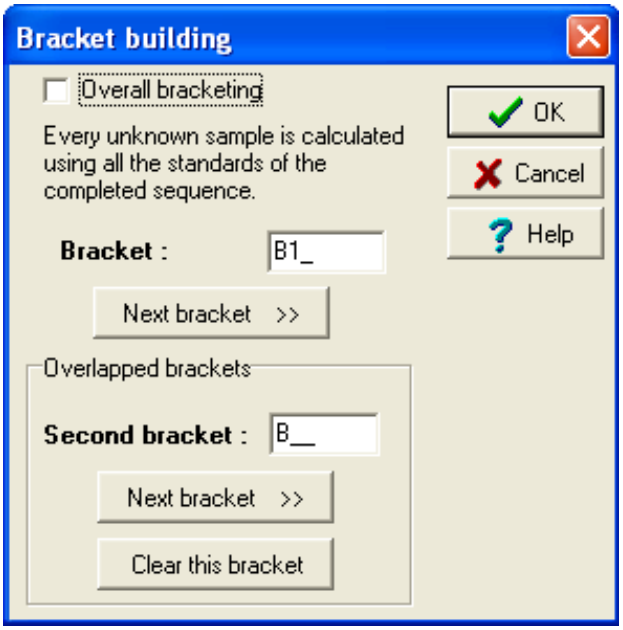
Run Suffix	Run ID	Standard	Level	Bracketing
Run	1	Standard	1	B1
Run	2	Standard	2	B1
Run	3	Unknown		B1
Run	4	Unknown		B1
Run	5	Standard	1	B1+B2
Run	6	Standard	2	B1+B2
Run	7	Unknown		B2
Run	8	Unknown		B2
Run	9	Standard	1	B2
Run	10	Standard	2	B2

The processing of the chromatograms acquired in sequence with bracketing is made after the acquisition of the whole sequence.

In the previous example the 10 injections are performed, then the calibration curve of the first bracketing is created with the four standard chromatograms Run1, Run2, Run5 and Run6. Then the first two unknown chromatograms (Run3 and Run4) are processed with this calibration curve.

This calibration curve is then archived and deleted and a second calibration curve is created with the four standard chromatograms Run5, Run6, Run9 and Run10. The last two unknown chromatograms (Run7 and Run8) are processed with this calibration curve.

To fill the bracketing column, enter the bracketing numbers separated with a ‘+’; for example ‘B1’, ‘B2’ or ‘B1+B2’ or use the button to access the following window:



This window allows you to easily fill in the bracketing column:

Check the 'Overall' bracketing box if the sample chromatograms should be created with a calibration curve containing all standards of the sequence.

Otherwise, for the first bracket enter B1_ and press the OK button. The cell is actualized with 'B1'.

Then for the second bracket, press the 'Next bracket >>' button. B1_ is changed in B2_ and press the OK button. The cell is actualized with 'B2'.

If the two brackets should overlay, press the 'Next bracket >>' button in the second bracket zone and press the OK button. The cell is actualized with 'B1+B2'.

NOTE: A maximum of 10 brackets can be defined. The use of bracketing is forbidden when using a multi-injector system or when selecting 'control sample' as sample type.

Use of System with a Prep-Ahead Sampler

If the system associated to the sequence is fitted out with a sampler which can prepare the sample to inject (mixing of sample, heating, stirring), a field allowing you to specify the maximum number of samples to prepare in advance is displayed above the grid of the sequence

.

Some restrictions are imposed in the sequence building and use:

- The same method must be defined for all lines
- The vials must be consecutive
- The same rack number must be defined for all lines
- Do not change the line order, add, delete insert or duplicate line, define multi injection per line or pause the sequence while it is running

NOTE: The preparation time of the sample is indicated in the Run Log of the chromatogram.

Running a Sequence

By pressing the Start icon, the sequence begins with the first acquisition.

It is possible to deactivate some of the acquisitions of the sequence by unchecking the 'Enable' cell of the corresponding lines.

If chromatograms already exist with the same file names, a warning message appears to inform the user that the files will be overwritten, or, if he does not own the corresponding right (profile defined in the Configuration Manager), forces him to change the chromatogram names.

When a sequence is started, the chromatograms are acquired one after the other in the defined order. The lines corresponding to chromatograms that are already acquired (or whose associated Enabled option is unchecked) are colored in green and the chromatogram that is being acquired is colored in yellow:

Injector2 | Injector1 | ALL

Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections
1	☑	test.METH	inj2-	1	30	1
1	☑	test.METH	inj1-	1	30	1
2	☑	test.METH	inj2-	2	30	1
2	☑	test.METH	inj1-	2	30	1
3	☑	test.METH	inj2-	3	30	1
3	☑	test.METH	inj1-	3	30	1
4	☑	test.METH	inj2-	4	30	1
4	☑	test.METH	inj1-	4	30	1
5	☑	test.METH	inj2-	5	30	1
5	☑	test.METH	inj1-	5	30	1

It is possible to insert additional acquisition lines (or modify existing lines) after the current chromatogram line that is being acquired (in yellow) during the sequence. Select the position of the new line to be inserted, and then click on the corresponding gray margin and select insert. A new line is inserted. To add a line at the end of the sequence, press . Fill it and the sequence lines will be acquired using the updated order. To remove a line, select it and press .

To insert an acquisition line just below the current line, it is better to first pause the sequence (icon). The current running sequence line continues until the specified acquisition time, but the next acquisition will not be started. To re-start the sequence, press the Start icon.

The Stop icon stops the sequence immediately.

To restart the sequence from the beginning, first press the Reset icon and then the Start icon .

NOTE: The sequence can be stopped automatically after a chromatogram process in case of Suitability test failure (see page 102), or Summary report variable test failure (warning or control) (see page 195). In both cases the user must have defined the 'Stop sequence' or 'Stop running sequence' action respectively for Suitability test and Summary report.

NOTE: If the user profile contains the right ‘Enable automatic save’, in the sequence section, a sequence file is automatically created each time a sequence was performed. This new sequence (which is a copy of the original one) is named sequencename_timestamp.SEQU (where sequencename is the name of the original sequence). This option has to be selected if the user wants to:

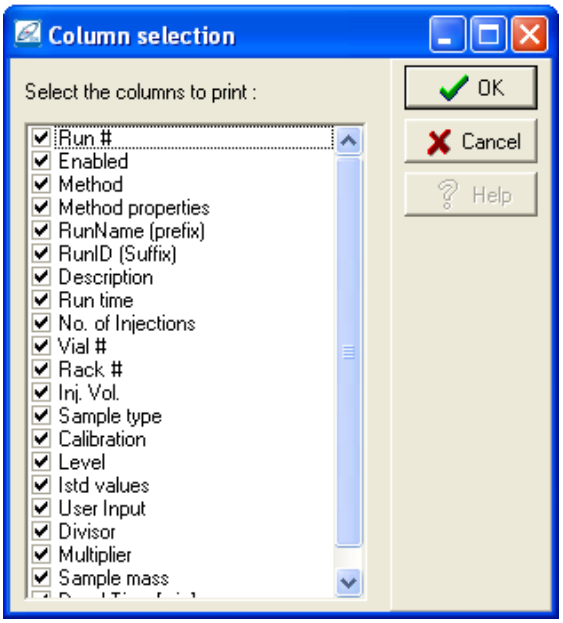
- sign a batch of chromatograms coming ‘from a sequence’

- create a REPL from a sequence, in the case a token was defined in the chromatogram name generation (acquisition parameter) (for example’ $Projectname-$AcqMethodName’, especially if the sequence was run as a remote sequence.

Printing a Sequence

When a sequence is opened and selected, press the icon or select the menu FILE / PRINT.

The following window appears:



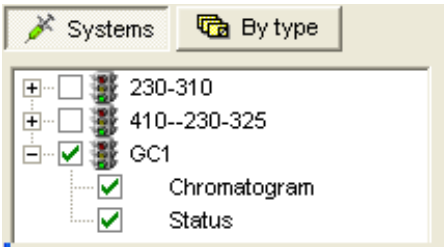
This window lists all the sequence columns. Check only the columns to be printed and press the OK button.

The sequence is printed.

Viewing an Acquisition

To view a chromatogram during its acquisition, select the ‘Systems’ tab. In the main screen, all the systems defined in the project in which user is connected are listed in the browser. If connected in “all projects”, all the systems defined in the group are listed.

In the browser, select the system(s) to view, the name is then preceded by and the selected system(s) is (are) automatically displayed. A tab is created for each new system in the right part of the screen. In the case of multi injector, visualization remains identical.



An idle system is preceded by the symbol, a system which is downloading the method or is waiting for the injection by , and a running system by .

To remove a view, uncheck the system performing the acquisition in the browser, the tab associated to the system is automatically removed.

Selecting the Information to Display

Select the “Systems” tab in the browser.

The acquisitions can be displayed system by system, or the same information can be displayed for several acquisitions on the same page.

Click on Systems to display all the information concerning an acquisition on a single page. Click on By type to display the information concerning the acquisitions according to type. (For example, all the chromatograms or the system status information, or both).

- System mode

In the browser, all systems that the user is allowed to control are listed (the list depends on the project of the user).

For each system, there are two sections: Chromatogram and Status.

If Chromatogram is checked for a particular system, a page is created containing the chromatogram. If Chromatogram and status for another system are checked, the new page will be separated between the section for the chromatogram and the section for the status.

- By type mode

There are two sections in the browser: Chromatogram and Status.

In each section (chromatogram and status), all systems which the user is allowed to control are listed.

If all the systems are checked, they will be displayed together. Four chromatograms can be displayed on each page, so if there are more than four selected systems, the other chromatograms will be displayed on a new page.

NOTE: It is best to not simultaneously view a large number of chromatograms or status. Doing so could lead to a problem with a virtual memory leak.

When “Status” is checked, information regarding the status of the acquisition system is displayed. The display will differ, depending upon the exact system configuration, e.g., whether the chromatograph is using full control drivers, etc.

If the system is not unchecked, and a new acquisition is started, the new acquisition will be displayed in the same window.

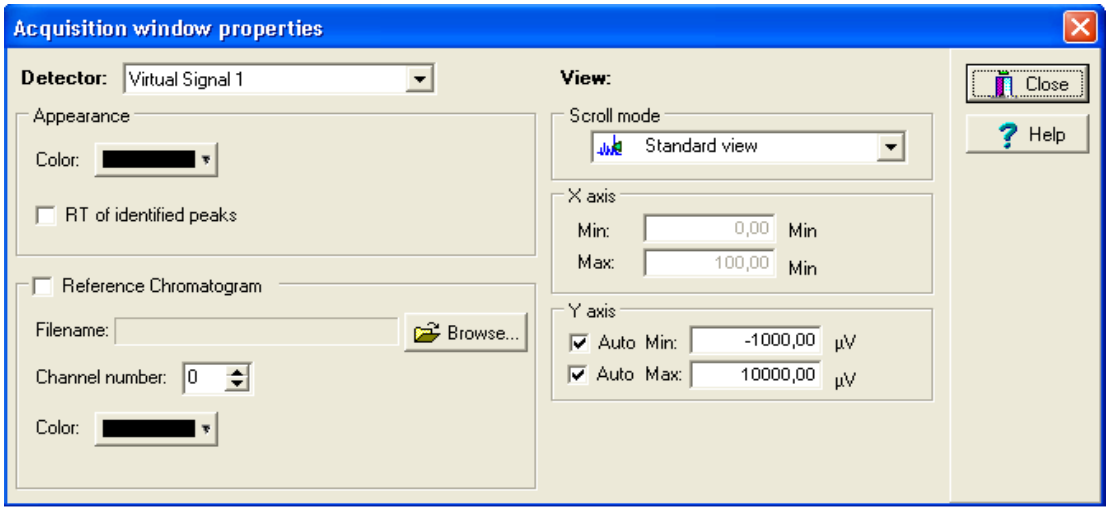
The Acquisition Window

The Tasks Bar

	Stops the current run. If the instrument is fully controlled, CompassCDS does not receive any information that the instrument is stopped. It is therefore necessary to stop the run within the software. CompassCDS will ask for a confirmation before stopping a run. Only the person who started an acquisition has the right to stop it, except some users that have the right to stop any running acquisition. This level of privilege is defined in CompassCDS Configuration Manager.
	Modifies the acquisition time. Note that by decreasing the acquisition time to a value less than the current run time, the acquisition will be stopped.
	Displays the chromatogram with automatic scaling: both scales are continuously updated after each acquisition points, such that the entire chromatogram is displayed.
	Displays the chromatogram in a fixed window. The parameters can be changed in the properties (see the corresponding icon below).
	Sets the parameters for the x-scale that moves along as the acquisition runs. It is possible to view only the last minute of acquisition, for example. To modify the width of this window, use the properties (see the corresponding icon below) and in the scrolling section, it is possible to change this default value.
	This icon is useful if there are several traces (several detectors) to stack the view of the two acquired chromatograms.
	This icon is useful if there are several traces (several detectors) to overlay the two acquired chromatograms.
	This icon synchronizes X axis of acquiring chromatograms. If one chromatogram is zoomed or moved, every chromatograms of the acquisition window will be also zoomed and moved.
	This icon modifies the acquisition view properties.

Acquisition View Properties

To look at the chromatogram viewing properties during acquisition, click on the icon. First, select the chromatogram to modify. The following window appears:

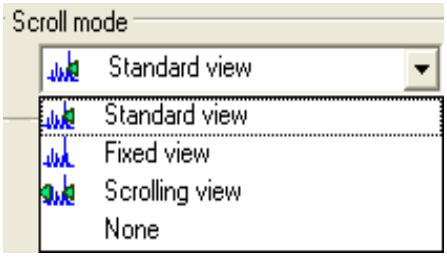


It is possible to define the colors of the chromatogram trace. To modify the colors of a trace, select the chromatogram channel to be modified in the 'Detector' zone, and then click on the color box to select the new color.

If peaks have been identified in the acquisition method (peaks identification section), it is possible to display their theoretical identification window on the chromatogram during acquisition. Select ‘RT of identified peaks’ option.

It is also possible to display a chromatogram as a reference. The new chromatogram will be overlaid with the reference. Press the Open icon ( ) and select the chromatogram to overlay in the Open file window and the chromatogram channel to overlay with the 1 box. To hide the reference chromatogram for a moment, uncheck the Reference chromatogram option.

- In the ‘Scroll mode’ zone, select the acquisition view:



Standard view: In this view, the X-scale is updated to the current acquisition time so that only the already acquired section is viewed. The Y- scale is automatic by default, but fixed limits can also be set (in the Y axis zone by un-checking the Auto option). An automatic scale means that the minimum is set to the minimum signal value and the maximum is set to the maximum signal value: the Y-scale is large enough to display all the acquisition points.

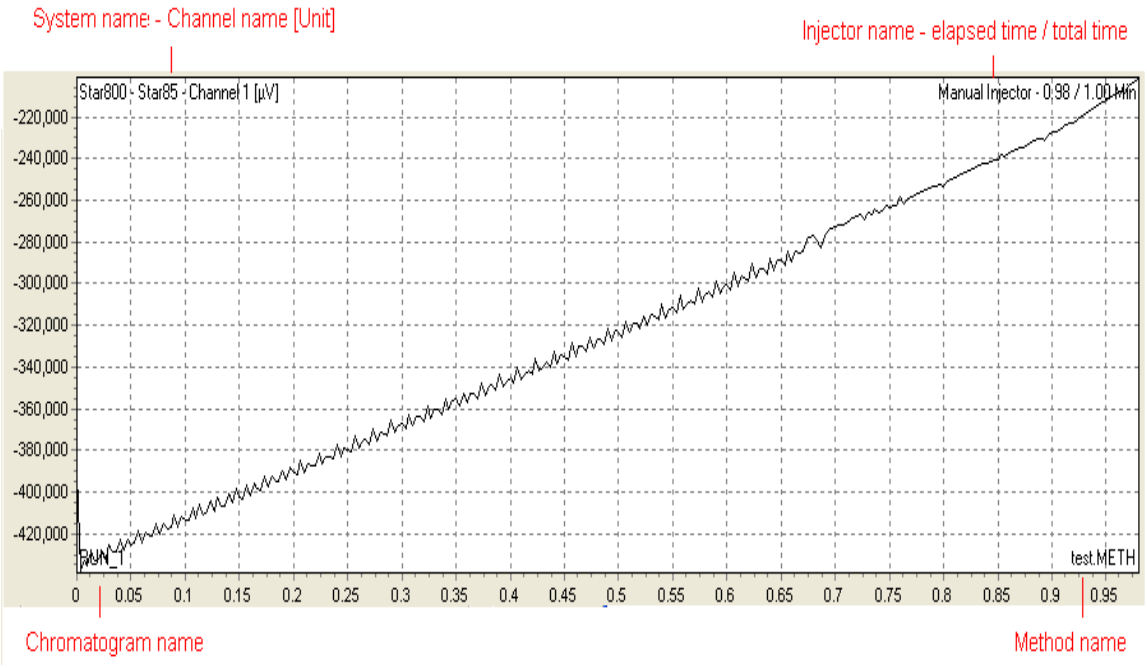
Fixed view: In this view, the X-scale is fixed, by default between zero and the expected acquisition time. The Y-scale is automatic by default, but if ‘Auto’ is unchecked, the corresponding values are set as fixed limits. The limits of the X-scale can be changed in the X axis field.

Scrolling view: This view shows only the last acquired points, within a width defined in the ‘Scrolling’ field. By default, the last acquired minute is shown. The Y-scale is either fixed or automatic.

Acquisition view display

Chromatogram plot and the following information are displayed on the acquisition view:

- System name - Channel name [Unit]
- Injector name – Elapsed time /total time
- Chromatogram name
- Method name



Acquisition Directory

It is possible to save the chromatograms in a different directory each day or in a directory depending on the instrument or user that performed the acquisition, etc. The special directories, which can be created to save the chromatograms, are called token.

For example you can start the same sequence with the same chromatograms every day but, save them in a directory named after the actual date.

Token mode is defined, thanks to a profile defined in the CompassCDS Configuration Manager.

Stop or Start a System

It is possible to stop or start a system from CompassCDS, as it is in CompassCDS Configuration Manager. The functions are available via the Systems tab: select a system and click on start or stop in the popup menu (double-click on the right mouse button). This option has to be set in the profile in CompassCDS Configuration Manager (Acquisitions / System properties / Allow to start or stop systems).

When stopping a system, the corresponding service is stopped, the system is idle. The start function starts the service associated to the system. It can be useful to stop a system without opening CompassCDS Configuration Manager, to carry out maintenance operations.

Exiting the CompassCDS Chromatography Data System

(While an Acquisition is running)

If a sequence is running, it is not possible to close CompassCDS. If Quick Start is actively running and CompassCDS is closed, the acquisition will continue and be saved, but will not be processed (note that the report will not be printed). The chromatogram will then be processed as soon as it will be opened within CompassCDS.

The Calibration Curves

A calibration curve consists of a series of individual calibration curves for each compound. The file is identified by a specific name.

For example, assume that there are three compounds in standard chromatograms, e.g. Glycine, Arginine, and Methionine, and the corresponding calibration curve is named ‘Amino Acids’. There will be a global calibration curve called ‘Amino Acids’, which will contain three calibration curves: one for ‘Glycine’, one for ‘Arginine’ and the last curve for ‘Methionine’.

Calibration curve Configuration

The calibration curve configuration is defined in CompassCDS Configuration Manager: the calibration curve can plot either quantities versus responses (area, height, area%, height%, $area^{1/2}$, and $height^{1/2}$) or responses versus quantities.

Building a Calibration Automatically

To create a calibration curve, the calibration method must be configured correctly (see page 76). Define at least the following parameters.

1. Select ‘Curve’ in the Factor list box.

   Specify the name of the calibration curve in the Calibration curve / File field and the unit of the standards in the Standard / Unit field.
   Complete the calibration table:

   Define the regression models and point-weighting mode.

   Define the number of compounds for each level in the standard sample table.

   When the method has been created and saved, it can be used to create calibration points.

2. If the standard chromatograms have already been acquired:

   Open the chromatograms to reprocess and then select the PROCESSING / REPROCESS menu. In the Reprocessing window, select the name of the first standard chromatogram and the name of the method.

   Now, select the appropriate calibration level from the calibration table column. This level should display the same standard amounts which correspond to the current sample standard amounts. Check ‘Clear old points’ to delete all the existing calibration points or check ‘Clear this level only’ to delete only those calibration points corresponding to the same calibration level. To add the calibration point to an existing curve, do not check anything. The cleared calibration points are not completely deleted, but archived.

   Now press ‘Reprocess’ to add the points.

Repeat the operations for all standard chromatograms (or use a reprocessing list, see page 173), take care to uncheck the boxes 'clear old points' or 'clear this level only' to add the next points, then close.

When the calibration curve has been created, open the Calibration page to view the results.

If the standard chromatograms have not been acquired:

Select the ACQUISITION / QUICK START menu options. Select the appropriate chromatograph and method, and then fill in the acquisition parameters in the Quick Start window.

In the Calibration section, select the appropriate calibration level, according to the values entered in the calibration table. Check ‘Clear old points’ to delete all the existing calibration points or check ‘Clear this level only’ to delete only those calibration points corresponding to the same calibration level. To add the calibration point to an existing curve, do not check anything. The cleared calibration points are not completely deleted, but archived.

The acquisition can now be started.

Repeat the operations for all the standard chromatograms and then close.

A calibration curve can also be created automatically during a sequence.

Building a Calibration Curve Manually

It is possible to add calibration points without using a standard chromatogram by entering point coordinates or by using a curve equation.

Open calibration curves, in the calibration point table, right click and select ADD POINT MANUALLY or ADD POINT FROM EQUATION. A window will appear which contains two tabs: ‘From equation’ and ‘manually’.

- Manual point addition.

  In the “Manually” page, select the number of points to be added.

  For each point, enter the response in the corresponding column and the amount in the other column.

  Select the calibration level corresponding to the points. The level will be useful if adding calibration points from a calibration chromatogram after the manual entries. If the level of the manually added point is X and ‘average level’ is checked in the method calibration part, this point is taken into account in the average calculation. When a level X point is added, if ‘Delete this level only’ is checked, the manually added point will be canceled.

  Press the OK button.

- Point addition from an equation:
- In the ‘From equation’ page, enter the curve equation from the drop-down list. Some existing linear equations are already entered for convenience. All that is needed is the replacement of the polynomial coefficients in the existing equations. The sign ‘^’ means ‘to the power of’

  Select the number of points to be added.

  For each point, enter the response or the quantity (according to the calibration curve orientation) in the corresponding column and then press Compute. The amount

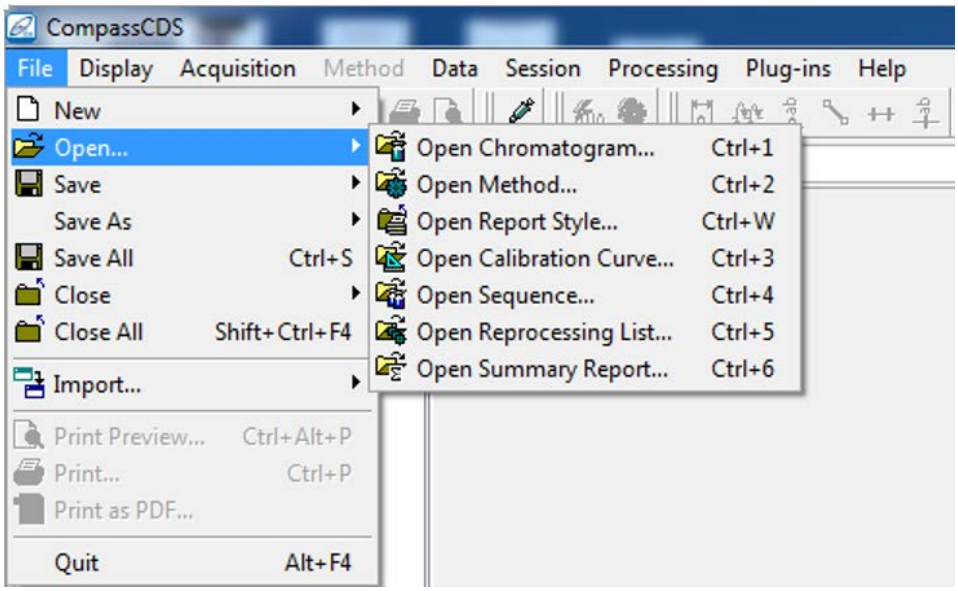
corresponding to the response in the equation is calculated, and displayed in the other column.

Select the calibration level corresponding to the points. The level will be useful if adding calibration points from a calibration chromatogram after the manual entries.

Press the OK button.

Displaying a Calibration Curve

To view a calibration curve, select the FILE / OPEN / OPEN CALIBRATION CURVE menu or use the icon “Open” and choose OPEN CALIBRATION CURVE in the sub menu.

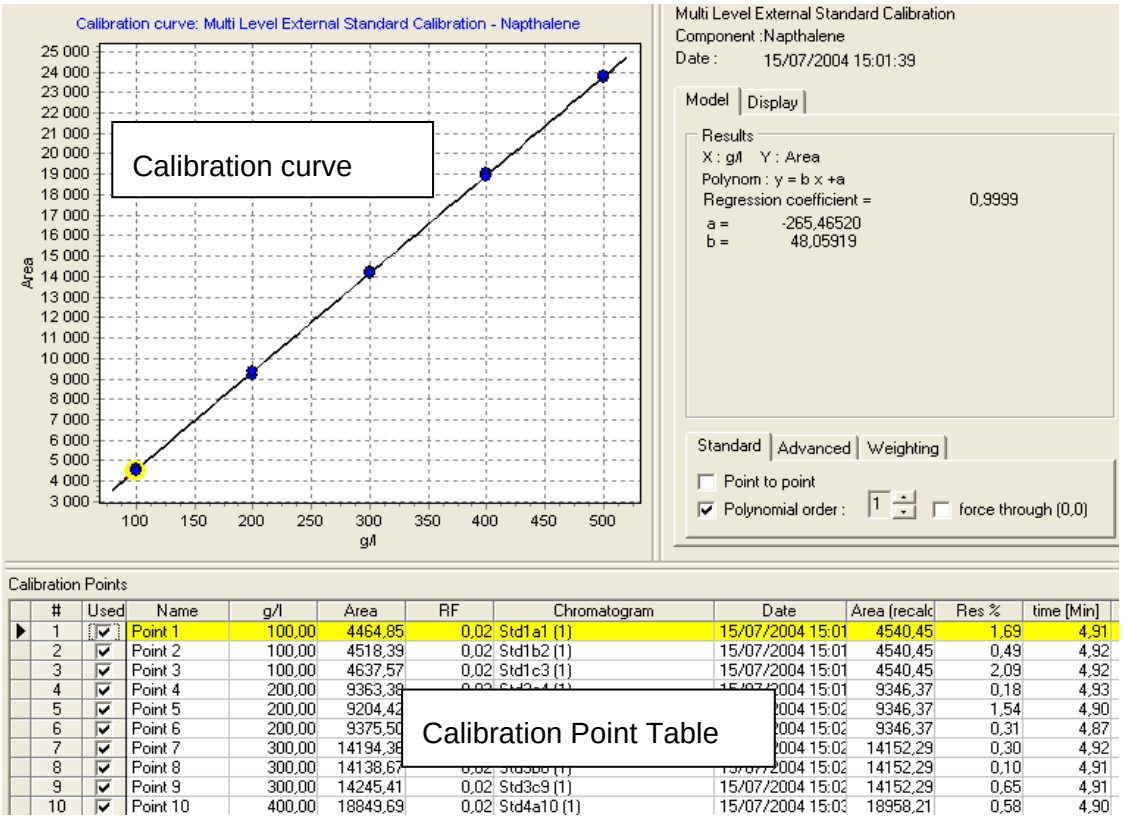


The calibration curves of all the compounds are listed in the browser.

When selecting a compound in the browser, the calibration curve of the corresponding component is displayed in the right panel.

Close to the plot are shown

- The global name of the curve, which is the file containing the calibration curves of every compound in the standard chromatogram.
- The name of the compound itself.
- The last date and time of modification.



#	Used	Name	g/l	Area	RF	Chromatogram	Date	Area (recalc	Res %	time [Min]
1	☑	Point 1	100,00	4464,85	0,02	Std1a1 (1)	15/07/2004 15:01	4540,45	1,69	4,91
2	☑	Point 2	100,00	4518,39	0,02	Std1b2 (1)	15/07/2004 15:01	4540,45	0,49	4,92
3	☑	Point 3	100,00	4637,57	0,02	Std1c3 (1)	15/07/2004 15:01	4540,45	2,09	4,92
4	☑	Point 4	200,00	9363,39			15/07/2004 15:01	9346,37	0,18	4,93
5	☑	Point 5	200,00	9204,42			2004 15:02	9346,37	1,54	4,90
6	☑	Point 6	200,00	9375,50			2004 15:02	9346,37	0,31	4,87
7	☑	Point 7	300,00	14194,36			2004 15:02	14152,29	0,30	4,92
8	☑	Point 8	300,00	14138,67			2004 15:02	14152,29	0,10	4,91
9	☑	Point 9	300,00	14245,41	0,02	Std3c9 (1)	15/07/2004 15:02	14152,29	0,65	4,91
10	☑	Point 10	400,00	18849,69	0,02	Std4a10 (1)	15/07/2004 15:03	18958,21	0,58	4,90

- The calibration curve

In this curve, the calibration points are shown and the regression model is drawn.

In this curve, as in chromatograms, both zoom in and zoom out functions are available. The curve may be copied to the Clipboard, and the graphic properties can be changed.

- It is possible to zoom in on the graphs by pressing the left mouse button in the top left-hand corner of the area to magnify and keeping it pressed until the bottom right-hand corner is reached.
- If the left mouse button is clicked, then dragged from the bottom right-hand to the top left-hand corners, the graph is brought back to full scale.
- A right mouse click within the graph area will display a popup menu with the following options:

Full scale: Returns graph to full scale.

Zoom in: Returns graph to the previous zoom in.

Zoom out: Returns graph to the previous zoom out.

Copy: Copies the curve as it appears on the screen (in order to paste it into another application using the local paste function).

Properties: Accesses the curve properties to modify its display.

NOTE: When the Average RF model is chosen, the curve shows the response factor (RF) versus the different calibration points (# point).

- The Model panel

The regression model is displayed in the Model panel with parameters quantifying the integrity of the regression. The regression model can be modified and the curve will be automatically recalculated.

- In the Model panel, the following elements are displayed:

The results, which are the theoretical equation of the regression curve, include the regression coefficient, and the numerical value of the equation coefficients (a, b, c, etc.)

NOTE-1: The method of least squares (or ordinary least squares) is used to calculate this regression coefficient.

The calculation is slightly different from the one in Excel®:

Excel®: $1-\frac{\sum(y-\hat{y})^2}{\sum(\bar{y}-y)^2}$

CompassCDS: $\frac{\sum(\hat{y}-\bar{y})^2}{\sum(\hat{y}-\bar{y})^2+\sum(y-\hat{y})^2}$

Where:

$\hat{y}$: is the standard deviation

$\bar{y}$: is the average

NOTE 2: If the Average RF model is chosen, the following curve related variables are displayed:

RF= Average response factor:

$$RF = \sum_{i=1}^{N} \frac{Q_i}{R_i}$$

RSD= Response factor_Standard deviation

$$RSD = \sqrt{\sum_{i=1}^{N} \frac{1}{N-1}\left(RF_i - RF\right)^2}$$

%RSD= Response factor_Relative Standard deviation

$$\%RSD = \frac{RSD \times 100}{RF}$$

N= the number of calibration points

It is possible to modify the regression model in this panel and to immediately view the results of the entire page (calculation of the regression curve and coefficient, curve display).

Different regression models are available:

Standard:

Point to point: The calibration curve is composed of lines drawn between the calibration points.

Polynomial: It is possible to modify the order of the polynomial. A calibration curve can be modeled with up to a 5th order polynomial. The polynomial regression can be forced through zero (for example, in case of a one-point calibration, the polynomial will be of order one and forced though zero).

If there are not enough points for the calculation (e.g. only one point available for a 2nd order polynomial), the order of the polynomial is reduced, and a message is displayed in the panel (below the polynomial coefficients).

It is possible to force the curve to go through (0, 0) by checking the corresponding option.

Advanced:

Power: this is a $\mathbf{y=ax^b}$ model.

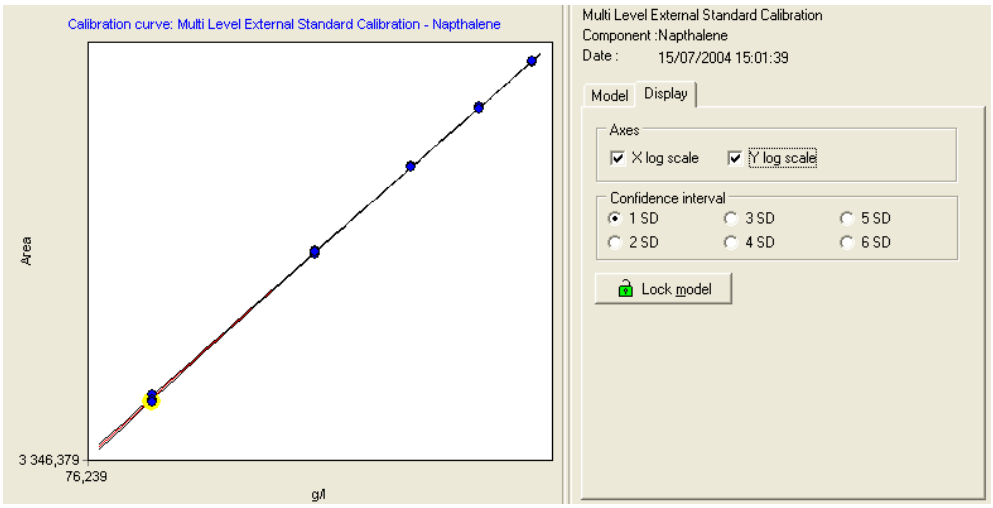
Exponential: this is a $y=a\ e^{bx}$ model.

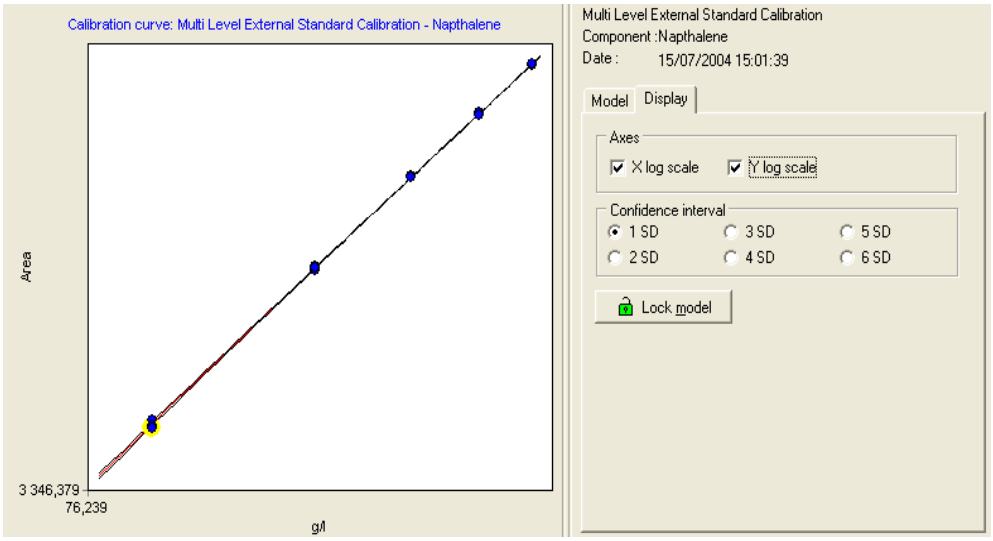
Logarithm: this is a y=a + b ln x model.

Average RF: If that model is chosen, it will imply automatically a linear model, force (0, 0) and $1/x^2$ weighting for the curve building. When the Averaged RF model is chosen, the other options which are set automatically cannot be changed until the calibration mode is changed.

- The Display panel

For both Standard and Advanced modes, it is possible to display the logarithm axis scales, by checking the X log scale or/and Y log scale boxes. These options can be interesting for curves for which the regression model is a power for example, it enables to view curve under a linear model, as displayed in the following example:





The confidence intervals can be chosen by the user (between 1 and 6 SD-Standard Deviation). Those intervals are displayed whatever the chosen model (linear, polynomial, etc.)

A Lock Model button can be found at the bottom of the panel. This locks the calibration curve after it has been validated.

Different weighting models are available:

None: This assigns the same importance to all calibration points.

x: This model calculates each calibration point using a weight proportional to the abscissa of the curve.

x^2: This model calculates each calibration point using a weight proportional to the square of the abscissa.

1/x: This model calculates each calibration point using a weight proportional to the inverse of the abscissa.

$1/x^2$: This model calculates each calibration point using a weight proportional to the square of the abscissa inverse.

log x: This model calculates each calibration point using a weight proportional to the decimal logarithm of the abscissa

ln x: This model calculates each calibration point using a weight proportional to the natural logarithm of the abscissa.

1-N: The weight of each new point is equal to the sum of previous point weights. For example, for 5 points, the weights are respectively: 1, 1, 2, 4, 8.

- The calibration points table

This is a table containing all calibration points with information about the source chromatogram and their addition.

#: Index

Used: Check or uncheck the boxes to activate or deactivate the calibration points.

Name: The name of the point corresponding to the order of addition.

Response: This column is the response (area or height) of the peak or the response of the compound divided by the response of the corresponding internal standard.

Quantity: This column is the compound amount or the compound amount divided by the corresponding internal standard amount.

RF: This column gives the response factor of the peak.

Chromatogram: This is the name of the source chromatogram from which the calibration point was added followed by its acquisition channel number in parenthesis. If the point was created manually, the cell content is “User defined”. If the point was added from a curve, the cell content is based on the curve equation.

Date: This column gives the point addition date and time.

Recalculated quantity: This column displays the projection of the calibration point where the quantity is recalculated to fall on the regression curve while maintaining the same response.

Res%: The residual standard percentage. It is calculated with the following formula:

$$\mathrm{Res\%} = \frac{y - \bar{y}}{y} \times 100$$

Where

y Is the quantity entered in the calibration table

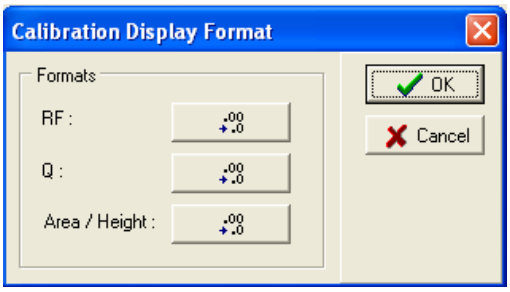
$\bar{y}$ Is the recalculated quantity

Time: The retention time of the peak corresponding to the compound in the standard chromatogram.

Level: The level defined in the calibration method. This is the level specified before the acquisition or the reprocessing

Username: The name of the user who created the calibration point.

NOTE: The format of the response factors, the response and the retention time can be modified. Right click in the calibration result table and choose the Format menu. The following screen appears:



Click on the variable you want to modify the format:

The new format is applied only in the calibration result table and in the Model panel for the RF.

- Activating and deactivating the points

Some calibration points can be far from the calibration curve (check the residual percentage). In this case, deactivate them, and the regression model is automatically recalculated without these points. Save the curve to use it for unknown samples.

There are two ways to deactivate or reactivate a point:

- In the calibration point table at the bottom of the panel, check or uncheck the “Used” boxes to activate or deactivate the calibration points. The last possibility is to double-click on the point in the browser.

A deactivated point is displayed in gray in the curve, the ‘Used’ box is unchecked in the calibration point table, and the icon is displayed in the browser.

An activated point is displayed in blue in the curve, the ‘Used’ box is checked in the calibration point table and the icon is displayed in the browser.

The Archives

Calibration curves are archived only if the corresponding profile has been associated with the user in the CompassCDS Configuration Manager (User profile, 21CFR11-user / Audit Trail / Archive Calibration Curve).

An archive is created, each time a point is added in the calibration curve.

The archives can be displayed either by component or by date.

Click on the

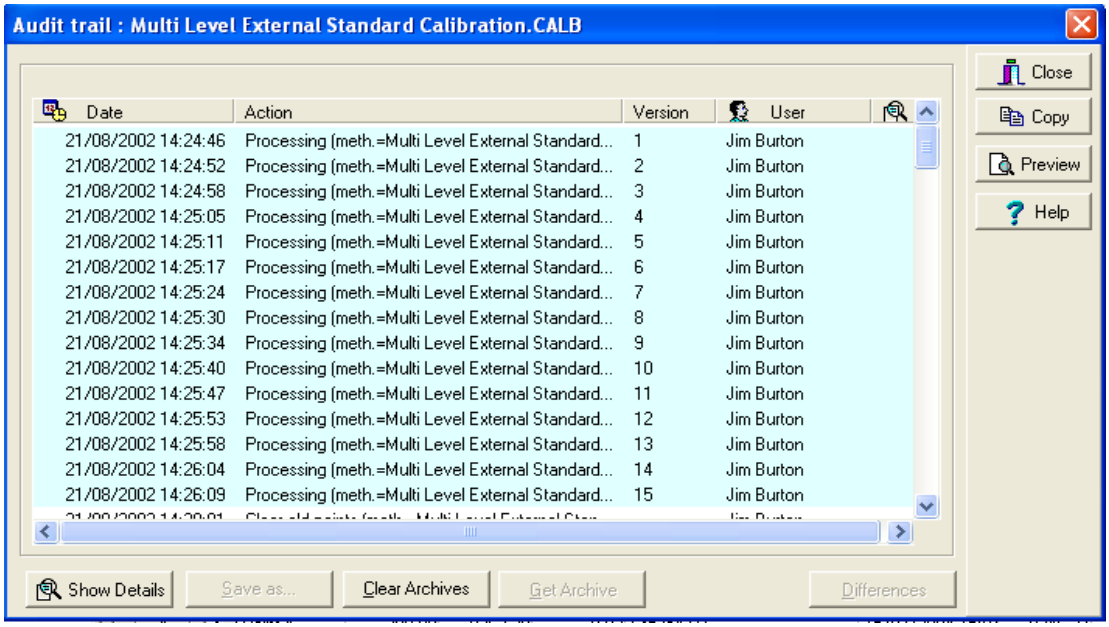
button to display them by component, or click on the

button to display them by date.

Click on the name or the date of the archives to display it in the right panel. The calibration curves are locked once they have been archived but the calibration point values and the regression model parameters can be viewed.

NOTE: The displayed archiving date does not correspond to the curve creation date but to the date on which it was replaced by another one, i.e., the curve creation date of the new calibration curve.

Note that an archived calibration curve can be used to reprocess chromatograms. Consult the Audit trail of the curve ( ):

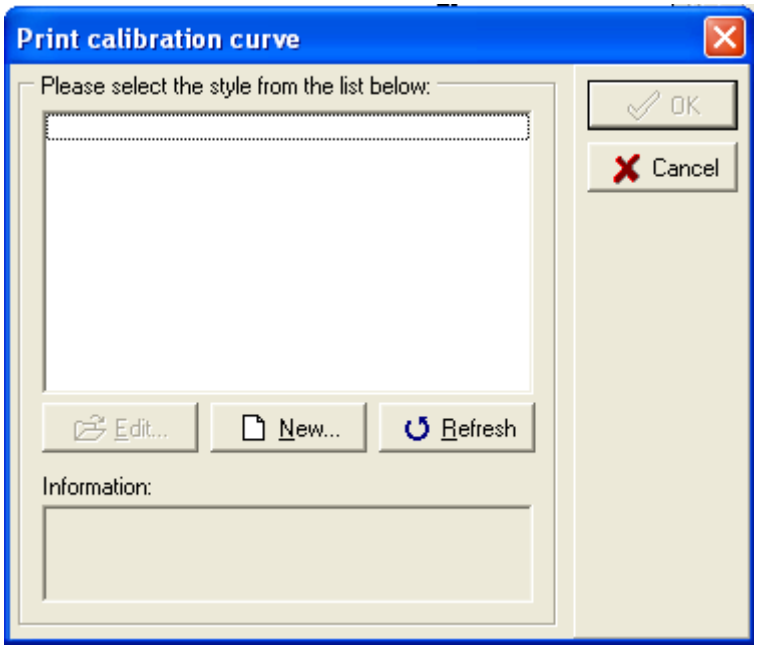

Audit trail : Multi Level External Standard Calibration.CALB
Close
Copy
Preview
Help
Date
Action
Version
User
21/08/2002 14:24:46 Processing (meth.=Multi Level External Standard... 1 Jim Burton
21/08/2002 14:24:52 Processing (meth.=Multi Level External Standard... 2 Jim Burton
21/08/2002 14:24:58 Processing (meth.=Multi Level External Standard... 3 Jim Burton
21/08/2002 14:25:05 Processing (meth.=Multi Level External Standard... 4 Jim Burton
21/08/2002 14:25:11 Processing (meth.=Multi Level External Standard... 5 Jim Burton
21/08/2002 14:25:17 Processing (meth.=Multi Level External Standard... 6 Jim Burton
21/08/2002 14:25:24 Processing (meth.=Multi Level External Standard... 7 Jim Burton
21/08/2002 14:25:30 Processing (meth.=Multi Level External Standard... 8 Jim Burton
21/08/2002 14:25:34 Processing (meth.=Multi Level External Standard... 9 Jim Burton
21/08/2002 14:25:40 Processing (meth.=Multi Level External Standard... 10 Jim Burton
21/08/2002 14:25:47 Processing (meth.=Multi Level External Standard... 11 Jim Burton
21/08/2002 14:25:53 Processing (meth.=Multi Level External Standard... 12 Jim Burton
21/08/2002 14:25:58 Processing (meth.=Multi Level External Standard... 13 Jim Burton
21/08/2002 14:26:04 Processing (meth.=Multi Level External Standard... 14 Jim Burton
21/08/2002 14:26:09 Processing (meth.=Multi Level External Standard... 15 Jim Burton
Show Details
Save as...
Clear Archives
Get Archive
Differences

Click on the Get archive button (if your profile allows you to do this operation). The current calibration curve is then replaced by the old one.

The user can also save a calibration curve archive under a new name thanks to the ‘Save as…’ option.

Printing a Calibration Curve

To print a calibration curve, open it then click on the icon. The following screen is displayed:



The user selects a defined report in the list, he can edit it by pressing the Edit button, create a new one by pressing the New button to customize the report, or refresh the list by pressing the Refresh button.

Manual Integration and Identification

Manual Identification

If the peaks are not well identified, it is possible to rename them manually within the peak report table (peak results).

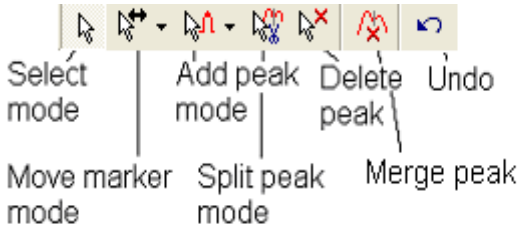
Double-click on the Name cell for the line of the peak to be renamed. Type the name of the peak in this cell.

If some reference peaks are identified manually the non-reference peaks will be identified according to the new reference times.

Manual Integration

The manual integration toolbar helps you to define the peaks manually (modify their start and stop time, delete or add…), the same modifications can be made within the peak results table, by changing manually the start and end retention times of peaks.

If the manual integration toolbar is hidden, select the DISPLAY / TOOLBARS menu and check Integration. The toolbar appears:



- Select mode

  This is the normal mode. If Select mode is pressed, it is possible to click on the markers in the graph to select them.

  Another possibility is to click on the corresponding peak in the peak result table.

  The third possibility is to press the right mouse button within the peak (in the graph), then choose PEAK / SELECT in the popup menu.

  The selected peak is highlighted in yellow in the peak result table, and its markers are highlighted in yellow in the graph.

- Move marker mode

  Press this icon to move a marker manually in the graph. Click on the marker to be moved, and then click a second time on the marker's new location on the graph.

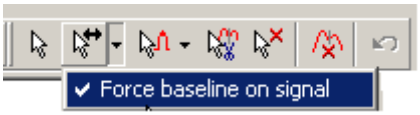
  Another possibility is to display the Start and End columns in the peak result table and to manually enter their new position.

  A marker cannot be moved before the previous marker or after the following marker.

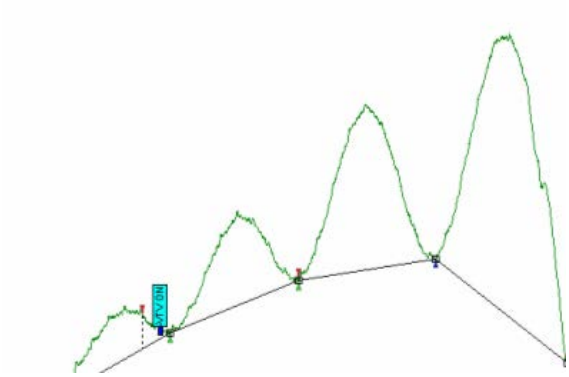
  Use the Move marker mode to move the integration events or the baseline. To move the baseline without the peak markers, hide the peak markers (press the display peak markers

icon) and move the markers symbolizing the edges of the baseline as for the other markers.

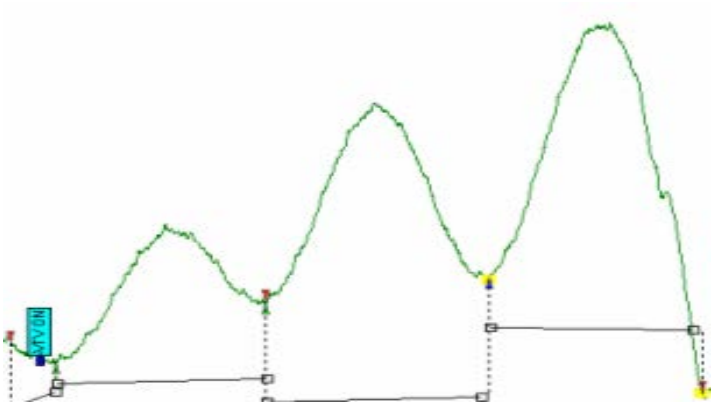
It is also possible to enforce or not the baseline on signal:



When the Force baseline on signal option is used, the baseline markers are always attached on the signal.



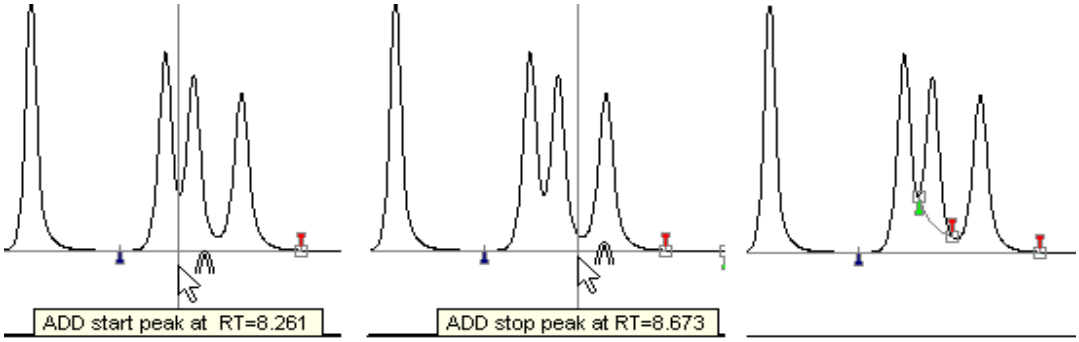
If that option is unchecked, it is possible to put the baseline marker wherever you want:



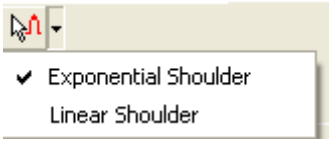
- Add peak mode

  Press this icon to add a peak. Click on the location of the start marker, and then click on the location of the end marker.

  If the two markers are added inside a peak, a shoulder peak is created:



The baseline of shoulder peaks is always a line, either exponential or linear. It is possible to define the shoulder integration mode (tangential or exponential) before moving markers, in the sub menu of the icon:



- Split peak mode

  Press this icon to split a peak. Click the left mouse button at the point where the peak should be split, and a valley marker is created at this location.

  Another possibility is to press the right mouse button at the point where the peak should be split, then select the PEAK / SPLIT option from the appearing popup menu.

  A shoulder peak (or a mother peak) can be manually split.

- Delete peak

  Select one peak (in the graph or in the table) as described above, then press the Delete peak icon.

  Another possibility is to first select the peak, then press the right mouse button within the peak result table, and select DELETE CURRENT PEAK from the popup menu.

  The peak that will be deleted using the two possibilities described above is the selected peak. This means that the peak highlighted in yellow within the peak result table and whose markers are highlighted in yellow within the graph is deleted.

  The third possibility is to press the right mouse button within the peak in the graph and then select PEAK /DELETE from the popup menu.

- Merge peaks mode

  Select one peak (in the graph or in the table) that as has been split into 2 peaks or that has a common marker with another peak (valley), then press the Merge peaks icon. The current peak is deleted and the next peak is extended to the left in order to include the deleted peak.

- Undo

  Press this icon to undo the previous manual action.

Manual Operation History

All the manual operations performed are listed in the chromatogram file.

Click on Results, then Manual operation in the browser to view the manual operation history displayed in the right panel.

The manual operations are either manual integration or manual identification.

The date and time of the operations are listed, along with the nature of the modification that was made.

Press the right mouse button in this panel and select UNDO LAST ACTION in the popup menu to cancel manual operations one after the other.

When saving a manually modified chromatogram, the manual operations are saved along with this history.

NOTE: It is possible to print the manual operation list in the report.

Modifications due to Manual Operations

When a peak is added or when the markers of a peak are moved, the variables are updated with the new response values.

But, if the chromatogram is a standard one, the modifications are not automatically taken into account. It will be necessary to create some calibration points with this chromatogram again, and to deactivate the previous ones. Enter the Reprocessing window to add the points (PROCESSING / REPROCESS) and open the calibration curve in the corresponding tab set (FILE / OPEN / OPEN CALIBRATION CURVE) to deactivate the points.

NOTE: To reprocess a chromatogram, without losing the manual integration, select the menu PROCESSING / REPROCESS, uncheck the Clear Manual Operation box in the options page and reprocess the chromatogram.

Reprocessing a Chromatogram

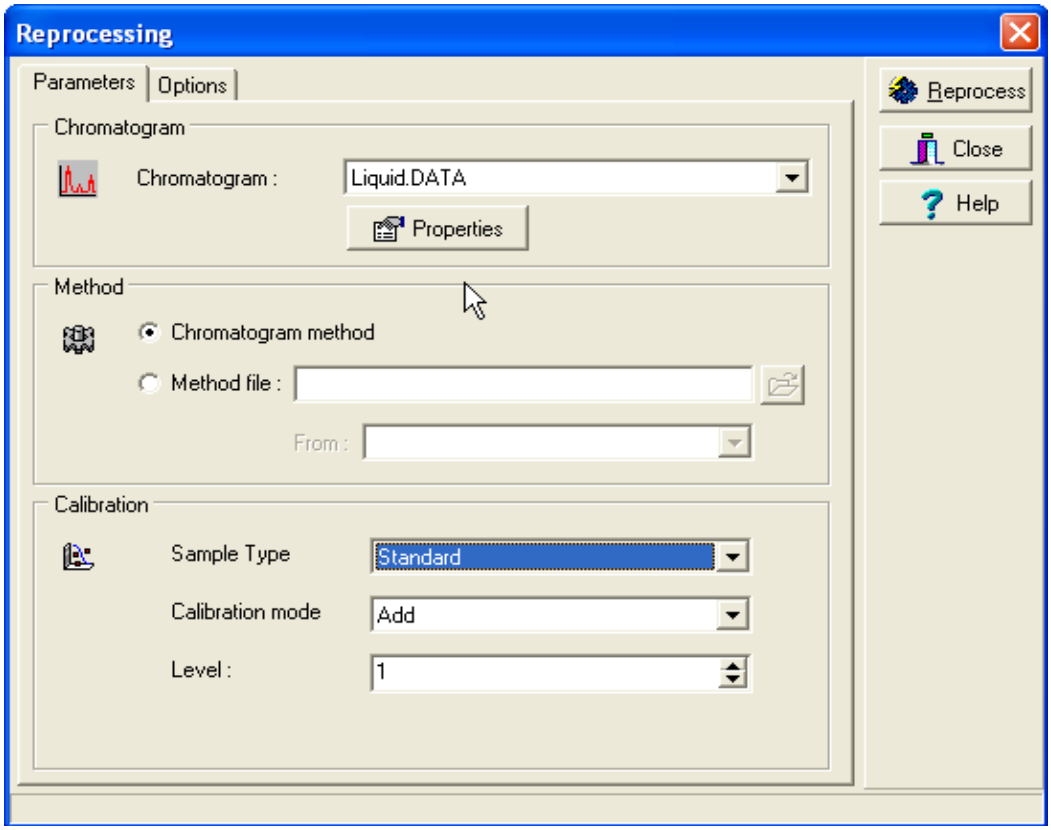
Once a chromatogram has been acquired, it is possible to reprocess it with another method. The previous method will not be lost but will be saved in the Audit Trail, if this function is defined in the CompassCDS Configuration Manager. For each processing or reprocessing a copy of the file is saved with the name of the user doing the processing. This file can be recovered (see Audit Trail page 204).

Single Reprocessing

The chromatogram should be opened in CompassCDS to be reprocessed in the single reprocessing window.

Choose the menu PROCESSING / REPROCESS to access the reprocessing window:

The 'Parameters' tab



In the Chromatogram zone, select the chromatogram file to reprocess from the list of all the chromatograms opened in CompassCDS.

If some properties of the chromatogram have to be changed before the reprocess (multiplier factor, divisor factor, sample mass, internal standard values, dead time) click on the Properties button and define the new values.

Then choose the method in the corresponding field. If 'Chromatogram method' is chosen, the method from the chromatogram file is used. If another method should be used, choose 'Method file' and press the open icon ( ) in order to choose a method.

In the Calibration section, define in the Sample Type field whether the chromatogram is a blank, an unknown, a standard, a control sample or a control sample of level-I. According to the option selected, the chromatogram process is different. In the Calibration mode field (available if the user is assigned the right to overwrite calibration curve) define whether the user will delete the existing curve and build a new one by selecting Clear old points, or erase only the points of the defined level by selecting Clear level only, or add the calibration point to an existing curve by selecting Add. Then define the level in the case of Standard or Control Sample (level-I) sample type selection.

NOTE: If the sample type is Control sample (level-I), and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level-I) in case of suitability test failure.

When the archive calibration curve profile is defined in CompassCDS Configuration Manager (21 CFR11 / Audit trail / archive calibration curve), it is possible to reprocess the chromatogram with the ‘unknown’ level either with the Calibration curve used to obtain the results saved in the chromatogram (possibly old ones), or with the last saved calibration curve. Select ‘Unknown’ in the level box, and ‘chromatogram curve’ or ‘current curve’ according to the case.

If the different versions of the curve are not archived, the chromatograms are always reprocessed with the current curve.

NOTE: If a multi-channels chromatogram has to be reprocessed, repeat the operation channel by channel, by selecting the corresponding channel in the ‘Chromatogram’ field. The channel is specified in parenthesis after the chromatogram name: RUN-1(1), RUN-1(2)…

The ‘Options’ tab

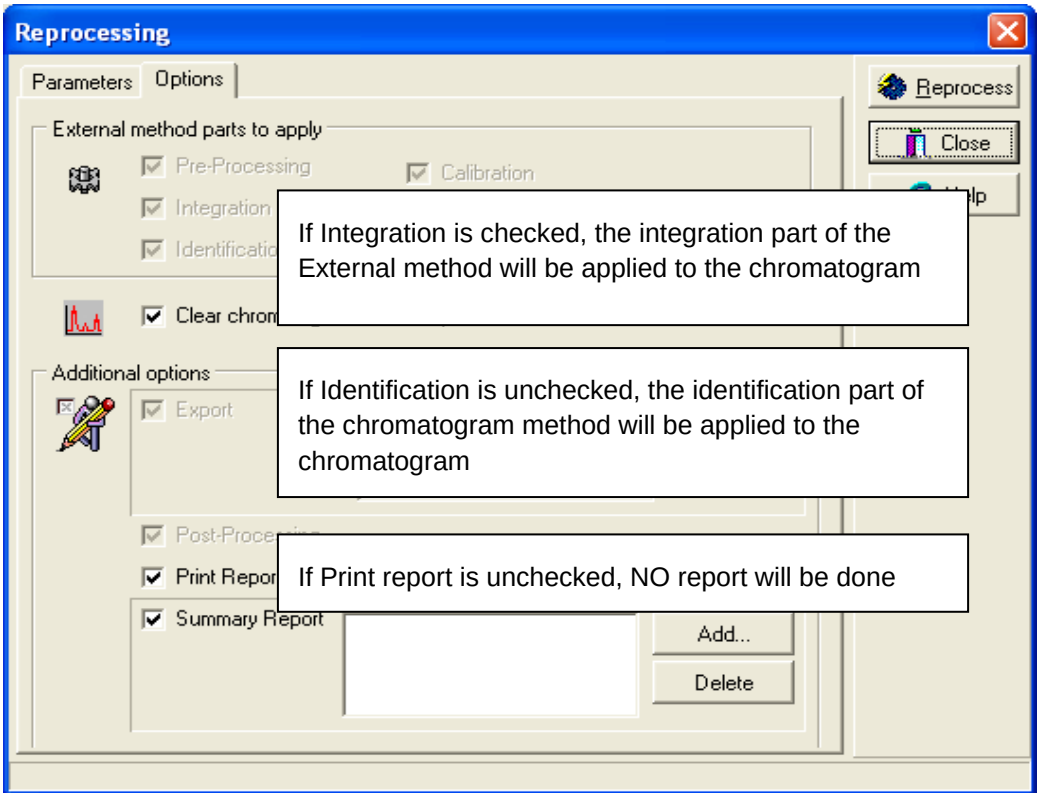
During the processing of a chromatogram, it is possible to deactivate certain processing functions. This can be useful in order to reprocess the chromatogram without printing a report for example.

When the chromatogram is reprocessed with its method, it is only possible to deactivate additional options (Export, Post processing, Print report and Summary report). It is not possible to deactivate the Preprocessing, integration, Identification, Calibration and suitability tests processes.

When the chromatogram is reprocessed with an external method, the Preprocessing, Integration, Identification, Calibration and suitability tests parts can come either from that external method (when the option is checked) or from the chromatogram method (when the option is unchecked). It is also possible to deactivate additional options (Export, Post processing, Print report and Summary report).

When the chromatogram is reprocessed, it is also possible to keep the manual operations already done on the chromatogram. To keep the manual operations, uncheck the option Clear chromatogram manual operations box.

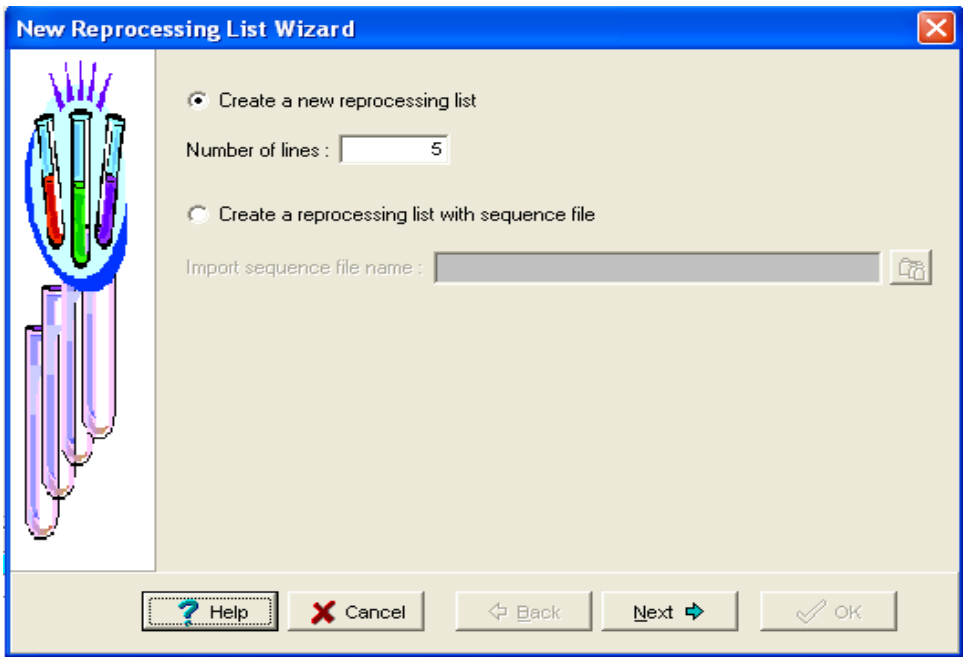
To access these options, choose the options page in the Reprocessing window.



Reprocessing Several Acquisitions: The Reprocessing List

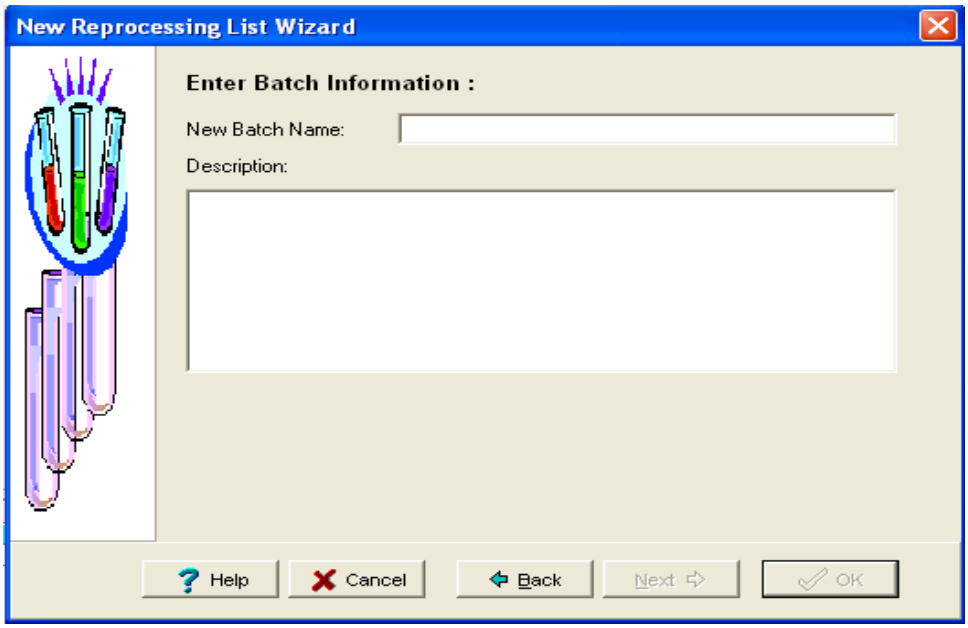
To reprocess several chromatograms rapidly, it is possible to create a reprocessing list.

Select the menu FILE / NEW / NEW REPROCESSING LIST**.** The following screen is displayed:



The user defines the number of lines of the reprocessing list, or if he wants to import chromatograms from a sequence, he has to check the second option and to select the sequence name.

Click on Next, the screen allowing the user to enter a name for the reprocessing list is displayed:



Enter a name and possibly a comment, and then click on OK. The corresponding reprocessing list is displayed.

The columns of the reprocessing list are very similar to the column of the sequence

In the “chromatogram name” column, select the name of the chromatogram(s) to be reprocessed: to open several chromatograms at the same time, press the ··· button of the first cell of this column. Then select all the chromatograms to be reprocessed with the combination of the left mouse button and the Ctrl and Shift keys. If there are more opened chromatograms than lines in the reprocessing list, lines are added at the end of the reprocessing list. Note that if selected chromatograms own several channels, one line is added by channel (by signal).

In the “chromatogram channel” column, select the chromatogram channel that should be processed: if the imported chromatogram owns 3 channels, three lines are added in the reprocessing list, with respectively the name of the detector 1, 2 and 3.

In the “method name” column, select the name of the method to apply. In the **“**method channel” one, select which channel of the method should be applied to (if the method is defined for more than one channel). Note that, when internal standards and/or user input variables are defined in the method they are imported. For example if a chromatogram has been processed with the default calibration method (area percentage), and an internal standard method is selected, the name of the internal standard(s) is imported in the ‘Istd’ column and the internal standard amount can be entered. Moreover, if a user input variable ‘A’ is defined in the chromatogram, and that this one is reprocessed with a method in which the same variable is defined, its value is kept.

In the “Method properties”, choose to apply parts either from the external method or from the chromatogram method. The Preprocessing, Integration, Identification, Calibration and suitability tests parts can come either from that external method (when the option is checked) or from the

chromatogram method (when the option is unchecked). It is also possible to deactivate additional options (Export, Post processing, Print report and Summary report).

It is also possible to keep the manual operations already done on the chromatogram. To keep the manual operations, uncheck the option Clear chromatogram manual operations box.

Values of the columns corresponding to variables saved in chromatograms (M, D, dead time, sample mass, user input, and Istd) are automatically imported from chromatograms. Nevertheless, if loading a method in which others user inputs and/or Istd are defined, the ones of the chromatogram are deleted. If common variables or Istd exist between chromatogram and method, the chromatogram values are kept.

In the ‘sample type’ column define if the sample is a standard, an unknown, a blank a control sample or a control sample (level-I).

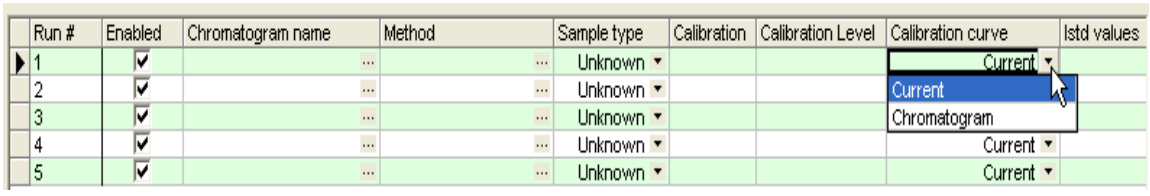
In the ‘calibration’ column, define for standard samples only, whether to keep the previous calibration points (Add), delete all the previous calibration points (Clear old points), or delete only those calibration points corresponding to the same calibration level (Clear level only). For standard samples, select the ‘calibration level’ corresponding to the quantities entered for those standards in the calibration table.

NOTE: If the sample type is Control sample (level I), and that in the method a suitability test is defined with the action ‘Modify calibration curve’, all the calibration points of the defined level will be replaced by the value of this control sample (level-I) in case of suitability test failure.

In the case of an internal standard calibration method, click on the ‘Istd values’ cell and press the ··· button, then enter the values.

Enter the User input variable values in the ‘User input’ column: click on the cell and press the ··· button, then enter the values.

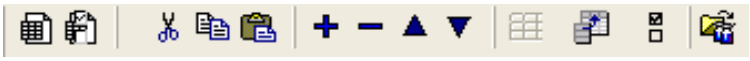
In the case that the calibration curves are archived (21 CFR11 / Audit trail / archive calibration curve), and that quantification has to be done, CompassCDS makes it possible to reprocess chromatograms either with the calibration curve used to obtain results saved in the chromatogram, or with the last archived curve. For this, precise in the ‘calibration curve’ column ‘current’ (to use the more recent curve) or ‘chromatogram’ (to use calibration curve corresponding to the saved results):



Caution: the calibration curve column only appears when the ‘Archive calibration curve’ profile has been defined in CompassCDS Configuration Manager, otherwise the chromatograms are always reprocessed with the current curve.

To work with bracketing, check the bracketing button (see page 151) to learn how to use this option in a reprocessing list).

The tool bar proposes the following options:



	This icon clears the content of all the cells of the reprocessing list
	This icon clears the unselected lines of the reprocessing list.
	This icon adds a line at the end of the reprocessing list.
	This icon deletes the selected line.
	This icon moves the selected line up.
	This icon moves the selected line down.
	This icon fills in several cells of the same column according to the content of the first one. For example, to fill in the 'Calibration level' column, select the cells to be filled in the column, then fill in the first cell with 1. Press this icon. A window appears in the workspace to define the increment between two consecutive cells. Press *OK*, and the cells are filled in. If the column contains a real value or the method, the content of the first cell is simply copied, then pasted in all others. Note that it is also possible to copy the content of a cell by selecting it, then put the mouse cursor to the left side of the cell, move the cursor down to the last cell the value must be copied, and select the fill block option in the popup menu.
	This icon permits selected columns to be hidden. Press this icon, and a window called 'Columns' appears. Unselect the columns to hide then click on OK. Be careful not to hide cells that must be filled in before the run.
	This icon allows the user to reprocess only the desired channel(s) of the listed chromatograms.
	This icon allows importation of all the chromatograms acquired in the same sequence in one step. The list of all the chromatograms of this sequence is added to the reprocessing list with the associated parameters saved in the chromatogram (M, D, dead time, mass, Istd, user input). If bracketing was defined in the imported sequence, the bracketing is kept. Of course the imported brackets can be modified afterwards.

When the reprocessing list is ready, press the start icon to run the processing. The lines are colored in green when the corresponding reprocessing has been completed. Once the entire list has been reprocessed, a message appears stating that it was "Completed".

NOTE: If defining "Blank" sample(s) in the sample type column, and use a method with a chromatogram name defined in the pre-processing part, the blank subtracted will be the one defined in the sample type column.

NOTE: It is possible to open directly a chromatogram belonging to a reprocessing list by double clicking on its name in the 'chromatogram name' column. To open several chromatograms, select the corresponding lines then choose the Open chromatogram(s) option from the context menu.

NOTE: In the case of several channels chromatogram, it is possible to uncheck the same channel(s) in all chromatograms of same structure in the total reprocessing list. In the enabled column, uncheck some channels of the first chromatogram (channel#2 in the following example):

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3

then select all the lines corresponding to the first chromatogram (for example the 3 lines in the case of 1 injectors/3 channels system):

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3

And click on the button. The pattern is applied to the entire reprocessing list:

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3
4	☑	1inj-3det-2.DATA	Virtual Signal 1 #1
5	☐	1inj-3det-2.DATA	Virtual Signal 1 #2
6	☑	1inj-3det-2.DATA	Virtual Signal 1 #3
7	☑	1inj-3det-3.DATA	Virtual Signal 1 #1
8	☐	1inj-3det-3.DATA	Virtual Signal 1 #2
9	☑	1inj-3det-3.DATA	Virtual Signal 1 #3
10	☑	1inj-3det-4.DATA	Virtual Signal 1 #1
11	☐	1inj-3det-4.DATA	Virtual Signal 1 #2
12	☑	1inj-3det-4.DATA	Virtual Signal 1 #3
13	☑	1inj-3det-5.DATA	Virtual Signal 1 #1
14	☐	1inj-3det-5.DATA	Virtual Signal 1 #2
15	☑	1inj-3det-5.DATA	Virtual Signal 1 #3

Viewing the Results

The results are saved in the chromatogram file.

To open a chromatogram, select the FILE / OPEN / OPEN CHROMATOGRAM menu, the icon or press together the Ctrl and 1 key. Select the chromatogram name(s) in the Open file window and press OK.

Integration Results Display on the Chromatogram

When the chromatogram is opened in CompassCDS its name appears in the browser. Click on Data to view the curve.

Chromatogram Scale

Once the curve is displayed in CompassCDS main screen, it is possible to magnify some parts of the chromatogram using the following two possibilities:

- Use the left mouse button: click on the top left hand corner of the area to be magnified and drag to the bottom right hand corner. Note that most of the time the width of the peaks should be emphasized more than their weight, so be careful to draw wide, but not very high rectangles.

NOTE: The chromatogram will be displayed in full scale again by clicking and dragging from any corner except the top left hand one.

- Use the popup menu (right click in the curve) options:

ZOOM IN emphasizes the curve and particularly if a zoom in has already been done, the same will be recovered.

ZOOM OUT minimizes the curve and particularly if a zoom out has already been done, the same will be recovered.

FULL SCALE returns the curve to full scale.

COPY copies the displayed chromatogram curve in order to paste it in other applications (Word, Excel, etc.).

PROPERTIES allow access to the properties to modify the display colors, view, etc...

To modify the chromatogram screen size, position the cursor between the two sections (chromatogram and method), the cursor will change to . Click and then move the limits of the display.

If the cursor is placed on the curve, the coordinates of the cursor are displayed in the status bar:

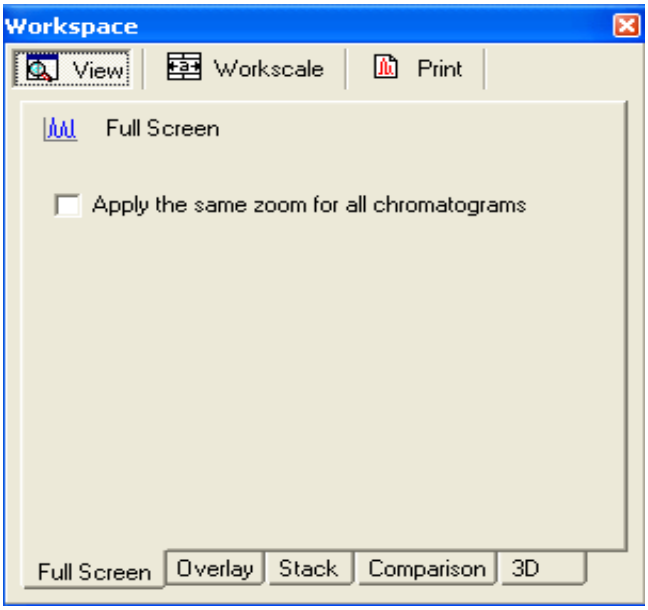
The cursor coordinates are shown after the name of the selected file.

The Workspace

The plotting of the chromatogram(s) can be modified in the workspace.

Press the icon to display the workspace.

- Select the 'View' screen to determine the display mode if several chromatograms are opened:



The following information will be displayed on each chromatogram, in the different display modes:

The X-scale and Y-scale units,

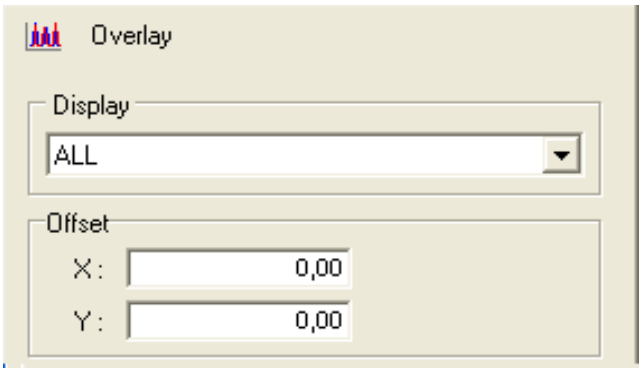
The chromatogram name with the same color as the corresponding plot,

Chromatogram annotations (peak annotations, event markers, peak markers, baselines…)

The active chromatogram name is surrounded.

FULL SCREEN: select the corresponding tab in the workspace screen or choose View / Full screen in the popup menu of the active chromatogram. In this mode, only the selected chromatogram is displayed. Click on the chromatogram name in the browser to display each curve one after the other. Check the 'Apply the same zoom for all chromatograms' option to display all the chromatograms with the same zoom.

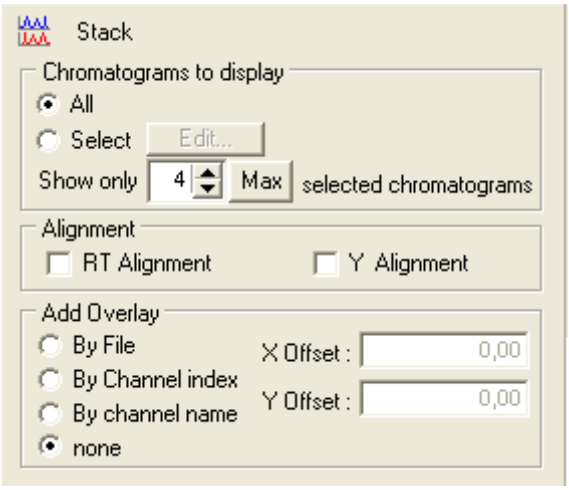
OVERLAY: Select the corresponding tab in the workspace screen or choose View / Overlay in the popup menu of the active chromatogram.



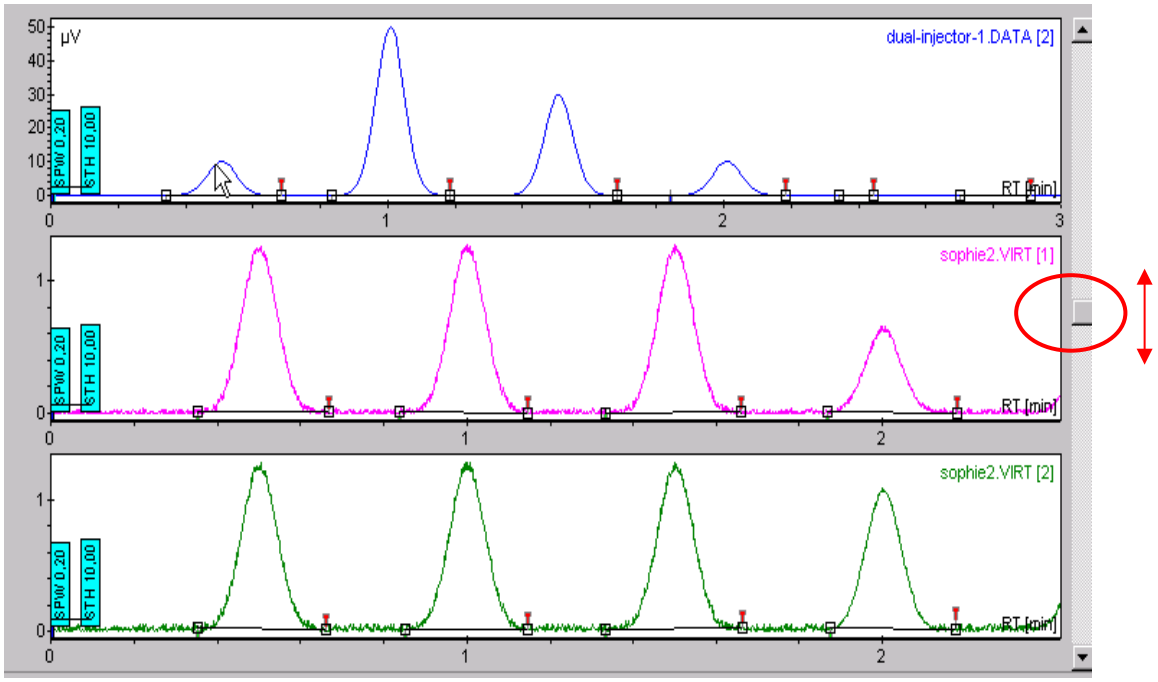
In this mode, the chromatograms are displayed in the same window. If the chromatograms are acquired on several channels (several detectors) it is possible to display only the chromatograms corresponding to the same detector. Select the required channel in the browser then choose the detector (channel) in the dropdown list. By default, ALL channels will be displayed and overlaid.

An X and/or Y offset can also be defined: the first open chromatogram will be the reference.

STACK: Select the corresponding tab in the workspace screen or choose View / Stack in the popup menu of the active chromatogram.



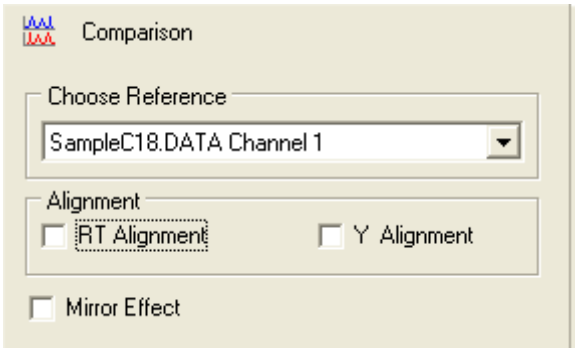
In this mode, several chromatograms are displayed in separate, stacked windows. If several chromatograms are opened, select the ones to stack in the 'Chromatogram to display' part. All the chromatograms are displayed by default, but you can also select the chromatograms to be stacked by choosing the Select option and pressing the *Edit* button. The user can also display only a few chromatograms among the selected ones, by selecting the number to display in the 'Show only X selected chromatograms' option. A scrolling bar appears which allows the display of the other selected chromatograms:



Check the RT Alignment AND/OR Y Alignment so that when zooming in on a chromatogram, or when moving it with the right mouse button, all the stacked chromatograms will be moved in the same way. To realize alignment on a defined chromatogram, select it in the browser.

If the chromatograms are acquired on several channels (several detectors) it is possible to overlay all the channels of the same chromatogram (BY FILE option) or all the chromatograms corresponding to the same channel (BY CHANNEL INDEX or CHANNEL NAME options), in the same view. ALL channels are stacked by default (no overlay): it corresponds to the NONE option.

COMPARISON: select the corresponding tab in the workspace screen or choose View / Comparison in the popup menu of the active chromatogram.

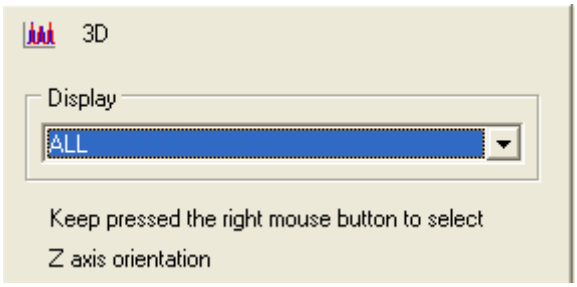


In this mode, only two chromatograms are stacked: the first one corresponds to the reference. If more than two chromatograms are opened, select the chromatogram to compare with the reference in the browser; it will be displayed in the second position, after the reference.

Check the RT Alignment AND/OR Y Alignment so that when zooming in on a chromatogram, or when moving it with the right mouse button, both chromatograms will be moved in the same way. To realize alignment on a defined chromatogram, select it in the browser.

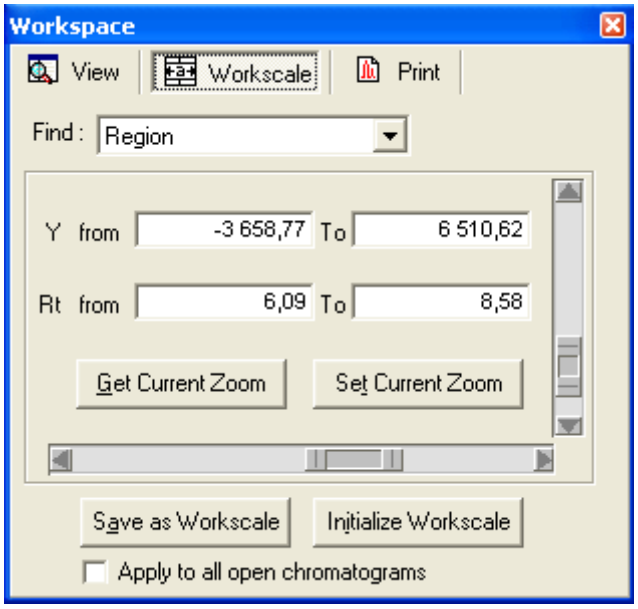
Check the *Mirror* effect option to invert the chromatogram to be compared with the reference (rotation through an angle of 180°).

3D: select the corresponding tab in the workspace screen or choose View / 3D in the popup menu of the active chromatogram.



In this mode, all the chromatograms are overlaid and can be shifted on a third axis: keep pressed the right mouse button to define the Z-axis orientation.

- Select the ‘Work scale’ tab to zoom on peaks or define manual zooms:



Select Find *Region* from the drop-down list to define manual zooms, then the limits in the Y and RT from -- to -- edit boxes can be defined. Press the Set current zoom button to apply these limits to the chromatogram.

Press the Get *current zoom* button to fill the edit boxes with chromatogram limits if the chromatogram was sized manually using the zoom in functions.

Use the scroll bars to zoom in the chromatogram: it is possible to reduce or increase the size of a bar by clicking one of its edges and dragging it. It is also possible to move them by clicking on their center and dragging them.

Select Find *Peak* from the drop-down list to zoom in on a peak: select the peak to be zoomed according to its name, index, area or height. Enter the corresponding name, index, area or height (for example ‘highest peak’) and then press the *Search* button to display the peak.

When a peak has been emphasized, use the Next and Previous buttons to view the other peaks.

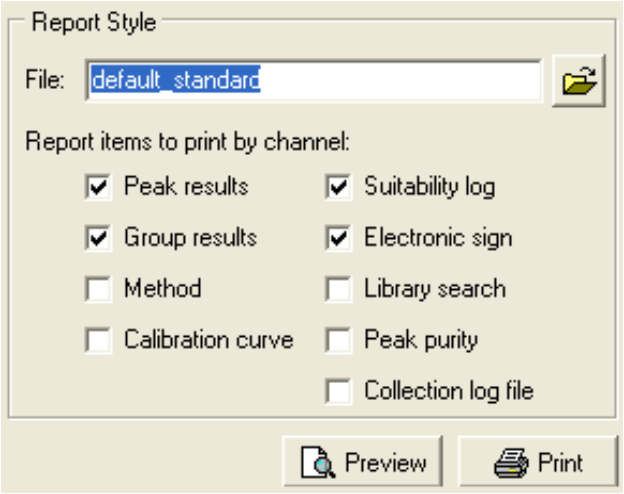
These page options can also be used to modify the working scale. The full scale is the maximum scale up permitted for zooming out. For example, if the chromatogram is composed of a huge solvent peak and many very small peaks, a full view of the solvent peak is not necessary therefore a scale to emphasize the small peaks should be defined. To set the working scale, zoom in on the chromatogram and press Save as work scale. Check the Apply to all open chromatograms box to apply this new scale to all the open chromatograms. If this work scale is customized for the channel-I of the chromatogram for instance, this customization will be applied to all channel-I of the open chromatograms only, if any.

If the working scale is not correct, press Initialize work scale to reset the working scale to the chromatogram acquisition scale.

Check the *Apply to all open chromatograms* box to reset the scale for all the open chromatograms. If this work scale is reset for the channel-I of the chromatogram for instance, this initialization will be applied to all channel-I of the open chromatograms only, if any.

NOTE: A scale defined with a manual zoom, in the WORK SCALE tab, is temporary, and is not saved in the chromatogram file when it is closed, whereas those defined and saved with the Save as work scale button will be saved in the chromatogram file.

- Select the 'Print' tab to print the results of the selected chromatograms in the same report. The following screen is displayed:



Select the report style to apply (previously built in CompassCDS Report Editor). Then select the objects to duplicate by chromatogram (one for each channel of each chromatogram). Chromatograms are printed as displayed on the screen.

Results Displayed in the Chromatogram

- **The markers:** The peak start and end are displayed with markers which can be customized. The default displayed symbols are:

Symbolizes a peak start marker: the time of the start marker is the value of the peak variable called 'Start'

- Symbolizes a peak end marker: the time of the end marker is the value of the peak variable called 'End'

Symbolizes a valley marker: this is a marker that indicates the end of a peak and the beginning of another one

Symbolizes a baseline end marker

NOTE: It is possible to select the symbol, color and markers size (Refer to page 99).

- The event annotations

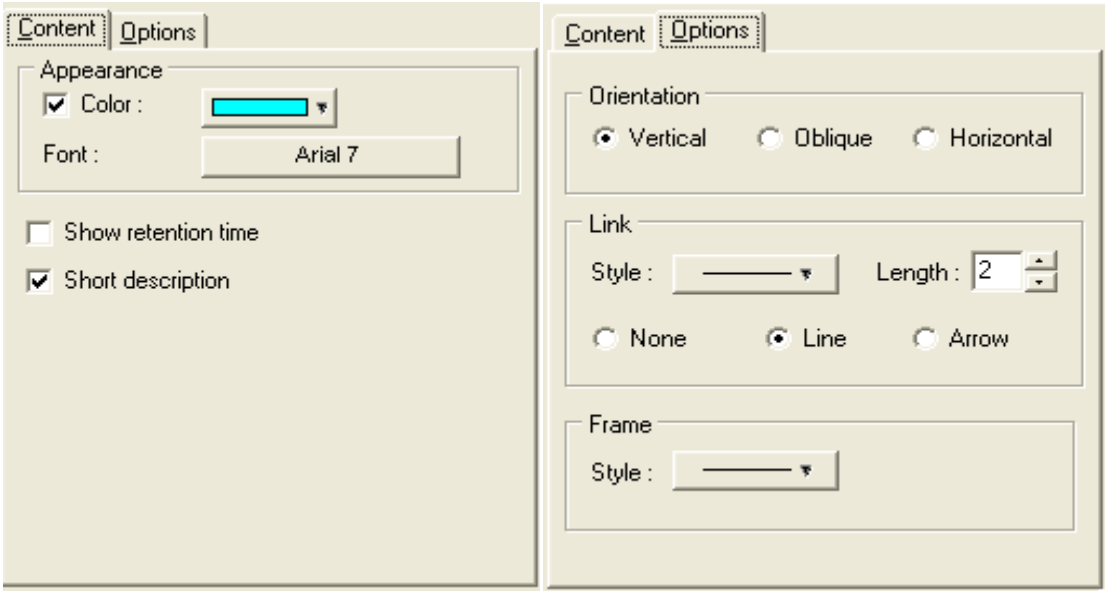
The events annotations display the integration events on the graph at the specified time.

It is possible to display or hide the integration events on the screen:

Press this button (Chromatogram annotation toolbar) to hide or show the event annotations.

Press this button (Chromatogram annotation toolbar) to hide or show the event markers.

Press this button (Display toolbar) to modify the display of event annotations. The displayed screen is divided into two sections: Content and Options.



NOTE: Those screens are also available from the Format / Chromatogram format part of the method, by selecting the Event annotations / Edit option.

In the Content tab, it is possible to modify the font and the background of the event annotations. The event description can be displayed as a code (DNP On will be displayed for Detect Negative Peaks On) by checking the 'Short description' option, or entirely by unchecking it. If Show retention time is checked in the Content page, the time when the event annotation is set, is displayed in the event annotation. For example: "1.25 DNP On" will be displayed if the Detect Negative Peaks On event was required at 1.25 minutes. Otherwise, only 'DNP On' will be displayed.

In the Options tab, define the Orientation of the annotations (Vertical, Oblique or Horizontal), the link parameters (line linking the chromatogram baseline to the event description) and eventually a frame.

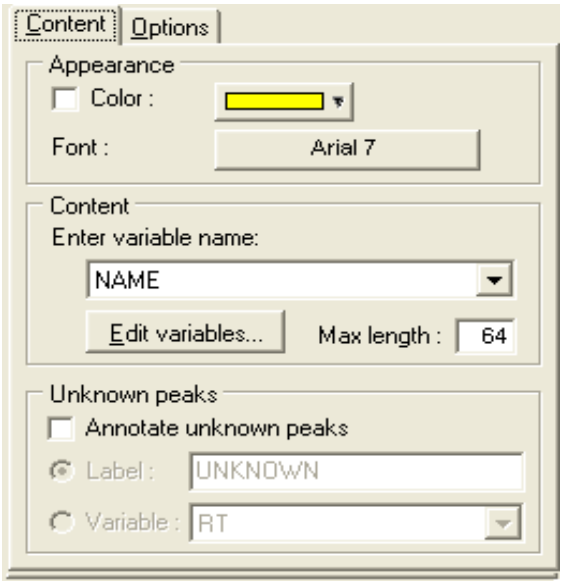
NOTE: To modify the event marker symbols, select the Properties option in the chromatogram context menu (or the Format / Chromatogram format part of the method) and select the Event markers / Customize button.

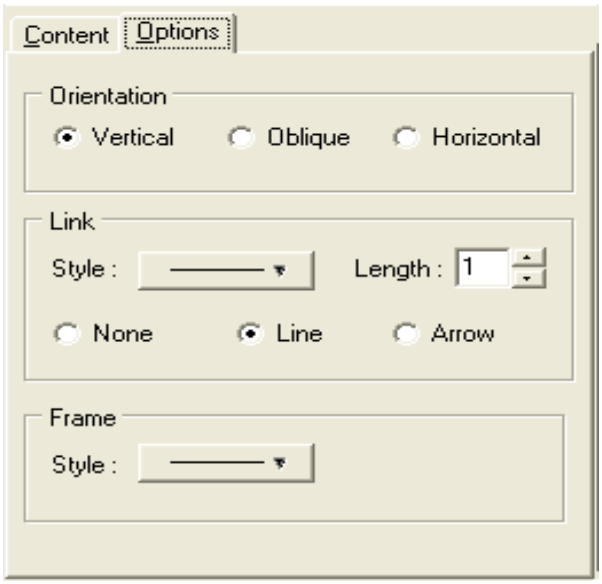
- Peak annotation

Peak annotation allows the displaying of information above each peak of the chromatogram. All the peak variables can be displayed.

Press this button (Peak annotation toolbar) to hide or show peak annotation.

Press this button (Display toolbar) to modify the display of peak annotation. The displayed screen is divided into two sections: Content and Options.





NOTE: Those screens are also available from the Format / Chromatogram format part of the method, by selecting the Peak annotations / Edit option.

In the Peak annotation window, the peak annotation display can be modified. The background color can be modified or removed. The font or orientation may also be changed.

In the Content tab, it is possible to modify the font and the background of the peak annotations. The content of the identified peak annotations can be changed and any variable defined in the variable editor (system peak variables, peak user input or peak user formula) can be displayed. To display a customized variable, grouping for example two or more variables, define a new peak user formula variable, as describe page 132).

If the annotation is too long, the user can define the number of characters to be displayed in the Max length field.

By default, no annotation is defined for unknown (non-identified) peaks. To annotate them, check the ‘Annotate unknown peaks’ option, and enter the label or choose the required variable in the drop down list.

In the Options tab, define the Orientation of the annotations (Vertical, Oblique or Horizontal), the link parameters (line linking the chromatogram baseline to the event description) and eventually a frame.

NOTE: To modify the event marker symbols, select the Properties option in the chromatogram context menu (or the Format / Chromatogram format part of the method) and select the Peak markers / Customize button.

Viewing the Peak and Group Result Calculation

The Result Tables

The results are displayed in a peak table and a group table. To view the results, click in the browser on the result section of the chromatogram channel to display.

- The Peak Table

Select the peak report item in the lower browser, and the peak table is displayed in the right panel.

Each line of the table represents a peak. When a line is selected, it is highlighted in yellow. The first and last peak markers of the corresponding peak are also highlighted in yellow in the graph.

The heading of the table columns is composed of the name and the unit of the variable. The name, the unit and the format of the variable can be modified in the variable screen. To access it, display the context menu of the desired column of the Result table and select the Edit variable X option.

At the bottom of the table, a line labeled Total is displayed in blue. The sums for all the peaks of the variables for which the total sum was required in the variable screen are displayed. The total area, height, area and height percentages, and quantities are calculated by default.

NOTE: CompassCDS can list the missing peaks in the result table, by indicating their name and theoretical retention times. The corresponding option has to be configured in the peak report format.

NOTE: CompassCDS displays areas only with positive values, i.e., if negative peaks are integrated their areas will still be positive values. To display the sign, add a column for the variable 'ISPOS' in the results table, if true is displayed the area is positive and if false is displayed the area is negative, or use the PEAKSIGN variable of the additional variables repository (see page137).

The Popup Menu:

In the peak table, press the right mouse button and a popup menu appears.

Choose ZOOM PEAK in this popup menu, and the selected peak will be highlighted in the chromatogram.

Choose COPY, and the peak table will be copied to the clipboard. Open any application (Excel is recommended), and use the local ‘Paste’ function to paste the peak report table into the application.

Choose DELETE CURRENT PEAK, and the currently selected peak is deleted (see also ‘Manual integration’).

Choose REPORT PROPERTIES to select the columns displayed in the table and modify their order.

Choose EDIT VARIABLE: XXX (in the column XXX), to edit the variable XXX and modify its format, its user name, etc.

- The Group Table

Select the group report in the browser, and the group table is displayed on the right panel.

Each line of the table represents a group. When a line is selected, it is highlighted in yellow.

The table column heading consists of the name and the unit for the variable. The name, the unit and the variable format can be modified in the variable screen. To access it, display the context menu of the desired column of the Group Result table and select the Edit variable X option.

At the bottom of the table, a line labeled, Total is displayed in blue. The sums for all the groups of the variables for which the sum total was required in the variable screen are displayed. The total area, height, area and height percentages, and quantities are calculated by default.

In the group table, press the right mouse button and a popup menu appears.

Choose COPY, and the group table will be copied into the clipboard. Open any application (Excel is recommended), and use the local ‘Paste’ function to paste the peak report table into the application.

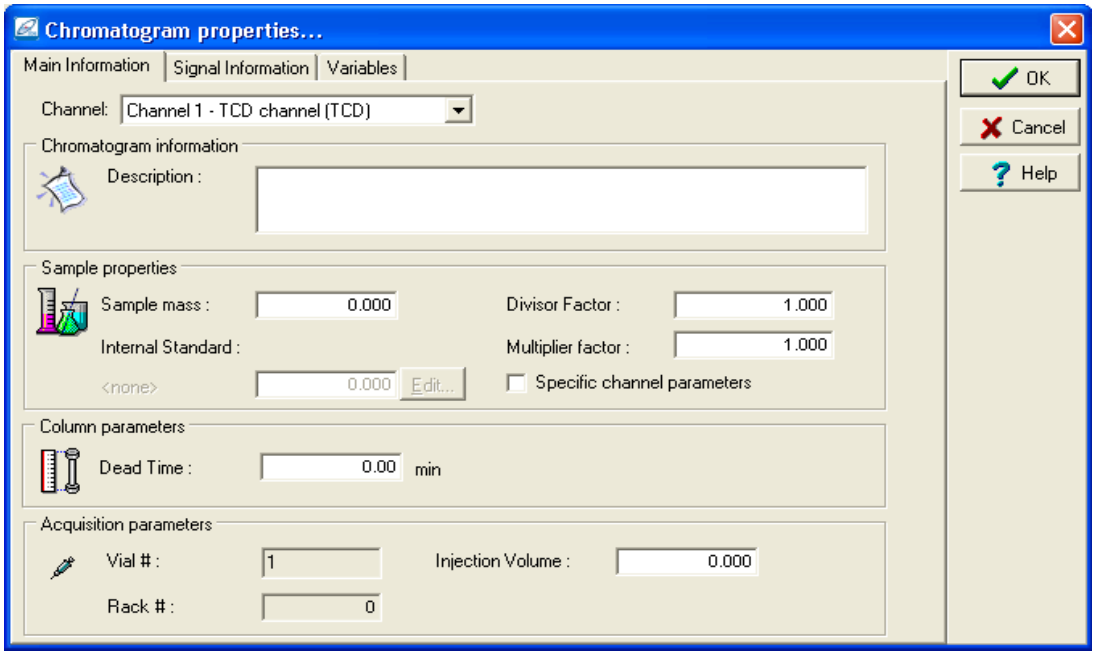
Choose REPORT PROPERTIES to select the columns displayed in the table and modify their order.

Choose EDIT VARIABLE: XXX (in the column XXX), to edit the variable XXX and modify its format, its name, etc.

NOTE: As for the peak and group result tables, the integration events, the chromatogram variable list, the calibration table, the identification peak and group tables can be copied and then pasted in Excel for example. Press the right mouse button in the corresponding table and select COPY in the popup menu.

Chromatogram Properties

To access chromatogram properties, first open a chromatogram and then select the DATA / CHROMATOGRAM PROPERTIES menu or the icon or press the F2 key. A three tab screen is displayed:



The Main information tab contains:

Chromatogram information: captured during chromatogram creation (either in the Quick Start screen or in the corresponding column of the sequence).

Sample properties: sample mass (mandatory if the result is expressed in mass% or mass ratio), divisor and multiplier (used in the quantification calculation), internal standard(s) quantity(ies), mandatory if the internal standard calibration type is selected, Specific channel parameters (except in the case of a system with one injector and one detector).

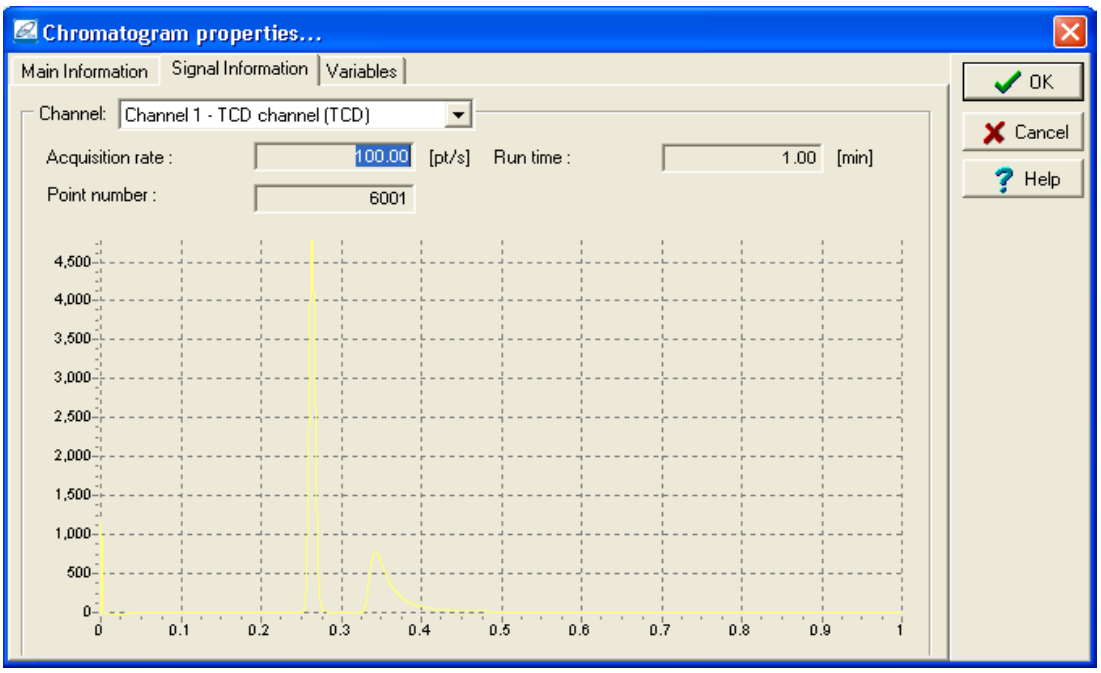
Column parameters: dead time (used for the selectivity and capacity factor calculation).

Acquisition parameters: vial and rack numbers, injection volume.

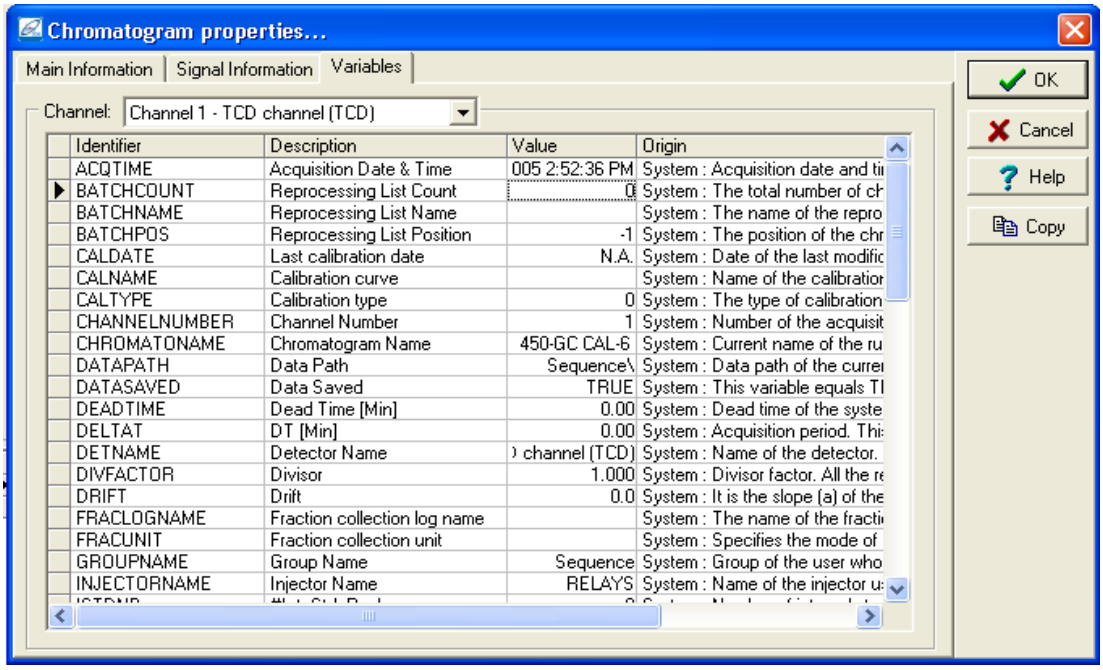
All fields except the acquisition parameters can be modified after the acquisition.

NOTE: When 'Specific channel parameters' is selected, user can select the channel name in the Channel field and complete the Sample Properties part by channel.

The Signal information tab brings together acquisition parameters: acquisition rate, run time and point number. These data are available by channel.



The Variables tab displays the value of system variables, calculated automatically for each chromatogram plus those of the global user input variables (see page 130). User input variables are displayed on a yellow background, the user can modify the values from this screen.


Chromatogram properties...
Main Information
Signal Information
Variables
OK
Cancel
Help
Copy
Channel: Channel 1 - TCD channel (TCD)
Identifier | Description | Value | Origin
ACQTIME | Acquisition Date & Time | 005 2:52:36 PM | System : Acquisition date and ti
BATCHCOUNT | Reprocessing List Count | 0 | System : The total number of ch
BATCHNAME | Reprocessing List Name | | System : The name of the repro
BATCHPOS | Reprocessing List Position | -1 | System : The position of the chr
CALDATE | Last calibration date | N.A. | System : Date of the last modific
CALNAME | Calibration curve | | System : Name of the calibratior
CALTYPE | Calibration type | 0 | System : The type of calibration
CHANNELNUMBER | Channel Number | 1 | System : Number of the acquisit
CHROMATONAME | Chromatogram Name | 450-GC CAL-6 | System : Current name of the ru
DATAPATH | Data Path | Sequence\ | System : Data path of the curre
DATASAVED | Data Saved | TRUE | System : This variable equals TI
DEADTIME | Dead Time [Min] | 0.00 | System : Dead time of the syste
DELTAT | DT [Min] | 0.00 | System : Acquisition period. This
DETNAME | Detector Name |) channel (TCD) | System : Name of the detector.
DIVFACTOR | Divisor | 1.000 | System : Divisor factor. All the re
DRIFT | Drift | 0.0 | System : It is the slope (a) of the
FRACLOGNAME | Fraction collection log name | | System : The name of the fracti
FRACUNIT | Fraction collection unit | | System : Specifies the mode of
GROUPNAME | Group Name | Sequence | System : Group of the user who
INJECTORNAME | Injector Name | RELAYS | System : Name of the injector u

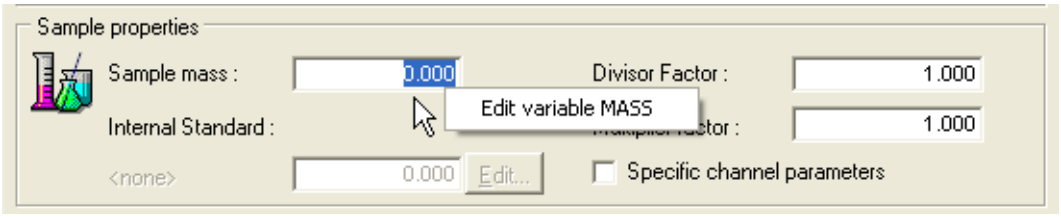
Note that it is possible to modify the format (number of significant digits, scientific format) of the following variables from this screen:

Main information tab: every variable of the ‘Sample Properties’ part and the internal standard(s) quantity (ies).

Signal Information tab: ‘Run time’ variable

Put the mouse cursor on the variable box, click on the right button, and in the popup menu select the Edit Variable XXX function, where XXX represents the variable name. The Variable Editor screen is displayed, allowing the change of selected variable format.

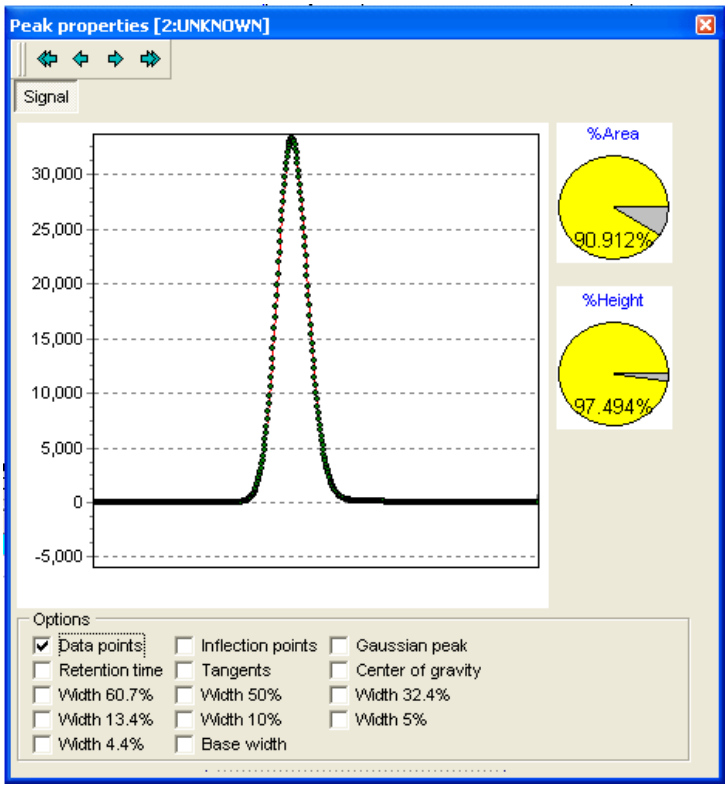
For example:



The Peak Properties

Click on to display the peak properties.

The peak properties provide an overview of the peak characteristics. Use the and arrows to scroll through the peaks.



The name of the peak is displayed as the window title. Press any of the options to view them for the selected peak. On the right of the screen, the area and height percentages of the peak are represented.

Of course, it is possible to emphasize or reduce the window size, to zoom in and out (using clicks and drags and the popup menu) within the graphics to view the details.

Click on the bar at the bottom of the screen to show or hide the options:

Printing the Results

A report can be printed automatically at the end of the acquisition. In the section of the method concerning the printed report, select a report style and the number of copies to be printed. To select a style, press the open button and choose the name of the style that will be used.

The report styles are created in CompassCDS Report Editor, the report creator. Select the FILE / NEW / NEW REPORT STYLE menu and refer to the CompassCDS Report Editor User's Guide or help file to create a report style.

To print a report manually, select the chromatogram to be printed, and press the Print icon or select the FILE / PRINT menu. A report will be printed for the chromatogram using the report style selected in the method. It is also possible to preview the report before printing using the FILE / PREVIEW menu or the Print preview icon.

If the chromatogram is not saved (displayed file different from the saved one), DATA NOT SAVED is written on the back of the report.

NOTE: The Printer Popup message can be disabled as follows: Start the Registry editor, and change HKEY_LOCAL_MACHINE\ SYSTEM\ CurrentControlSet\ Control\ Print\ Providers and set the entry NetPopup to 0. You should then reboot Windows (however stopping and restarting the print spooler will be sufficient). If the printer is on an NT server, then this setting needs to be set on the Server that controls the printed queue.

This can also be done from the Printers Control applet: Start the Printer control applet (Start - Settings - Printers); select "Server Properties" from the File menu then select the advanced tab, uncheck the "Notify when remote documents are printed". Click OK and reboot the computer.

Summary Report

The summary report provides the capability to monitor result(s) over a user-defined time interval.

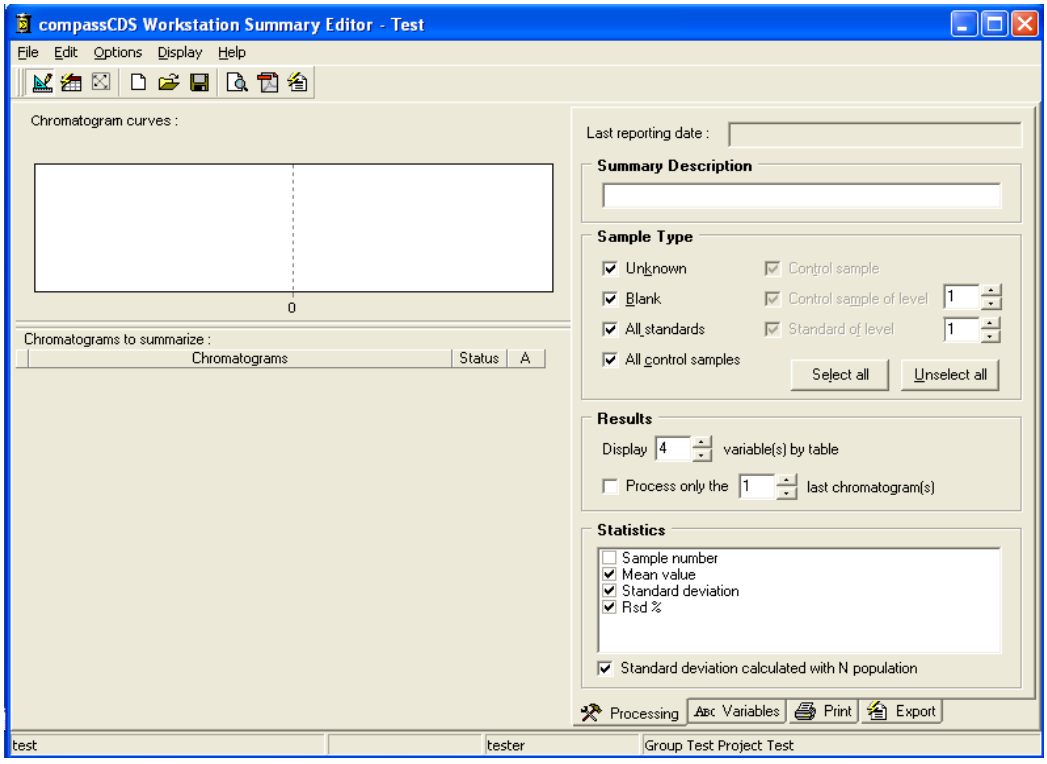
The summary report is similar to the reports created in the CompassCDS Report Editor. First, define a report style that determines what will be printed or edited and how this will be done.

Defining the Summary Report Format:

Select the FILE / NEW / NEW SUMMARY REPORT menu to access CompassCDS Summary Editor.

Processing

Select the processing tab:



On this page, select the type of chromatograms to be added automatically in the summary report and the type of statistics to be displayed in the result part.

A choice between adding Unknown, Blank, All standards or Standards of a defined level, All Control samples or only Control samples or Control sample of level is proposed. These features allow you

to filter the chromatograms to add in the summary report, when a large number of chromatograms are automatically sent.

It is possible to use only the X last added chromatograms to perform calculation, by checking the Enable the X last chromatogram(s) option where X is the desired chromatogram number.

The summary report generated consists in part of graphs and tables tracing the evolution of the variable(s). It is possible to define the variable number to display by graph/table, in the Show X variable(s) by table option.

Then define in the statistics section the calculation to realize:

Sample number: the number of chromatograms that have been added to the summary.

Mean: the mean value of the variables in the chromatograms. Note that if the variable is not calculated in a chromatogram, the mean value is not considered (i.e., its value is not considered to be zero).

Standard deviation: the standard deviation around the mean value is calculated as follows:

$s_x = \sqrt{V_x} = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n}}$ If the “standard deviation calculated with N population” option is checked

$s_x = \sqrt{V_x} = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n - 1}}$ if the option is unchecked.

Note: $\sum (x_i - \overline{x}_i)^2 = \sum ({x_i}^2) - \frac{\left(\sum (x_i)\right)^2}{n}$

Where:

x is the value of the variable in a chromatogram,

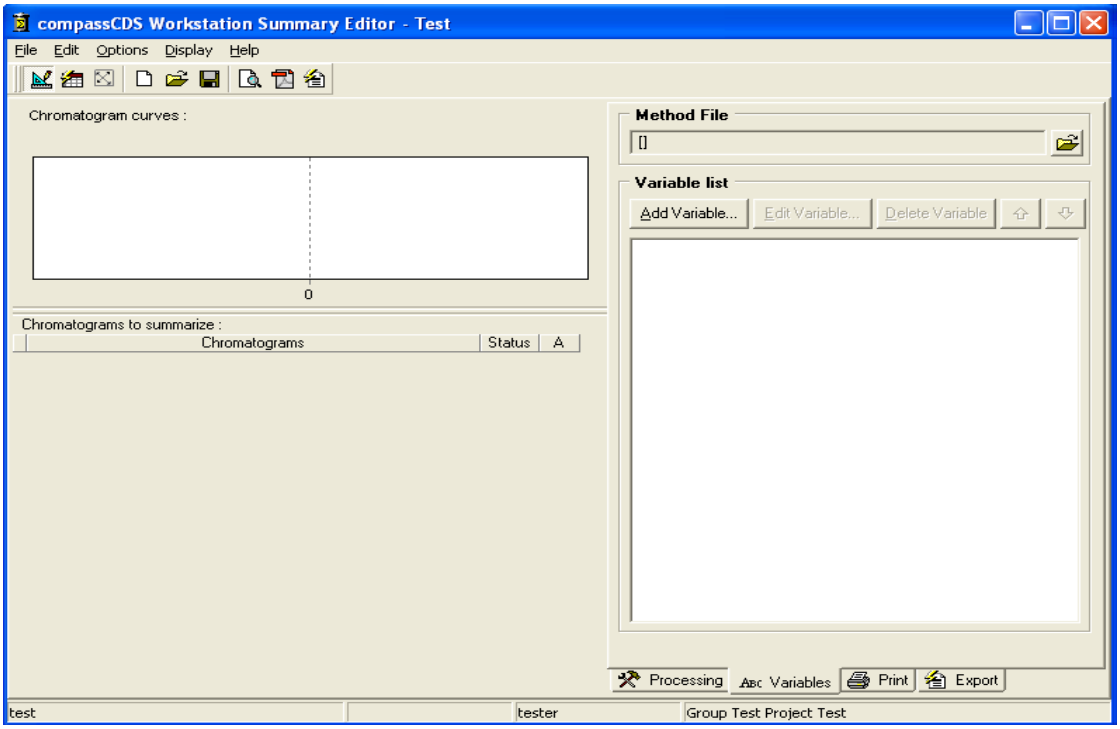
$\overline{x}$ is the mean value of the variable for all the chromatograms

n is the point number.

Residual standard deviation percentage: it is the standard deviation around the mean value divided by the mean value and multiplied by 100:

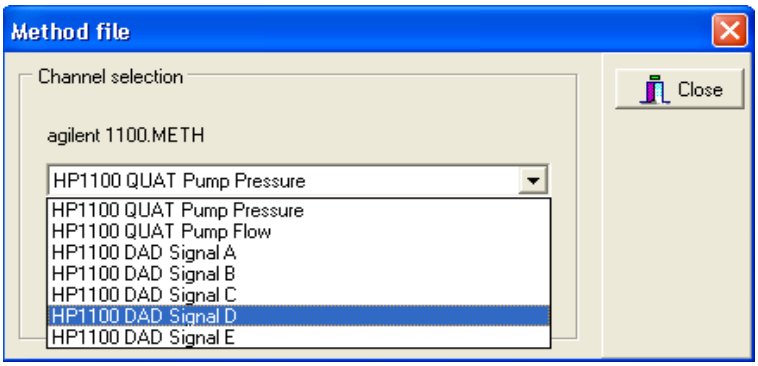
Variables

Select the Variables tab. The following screen is displayed:

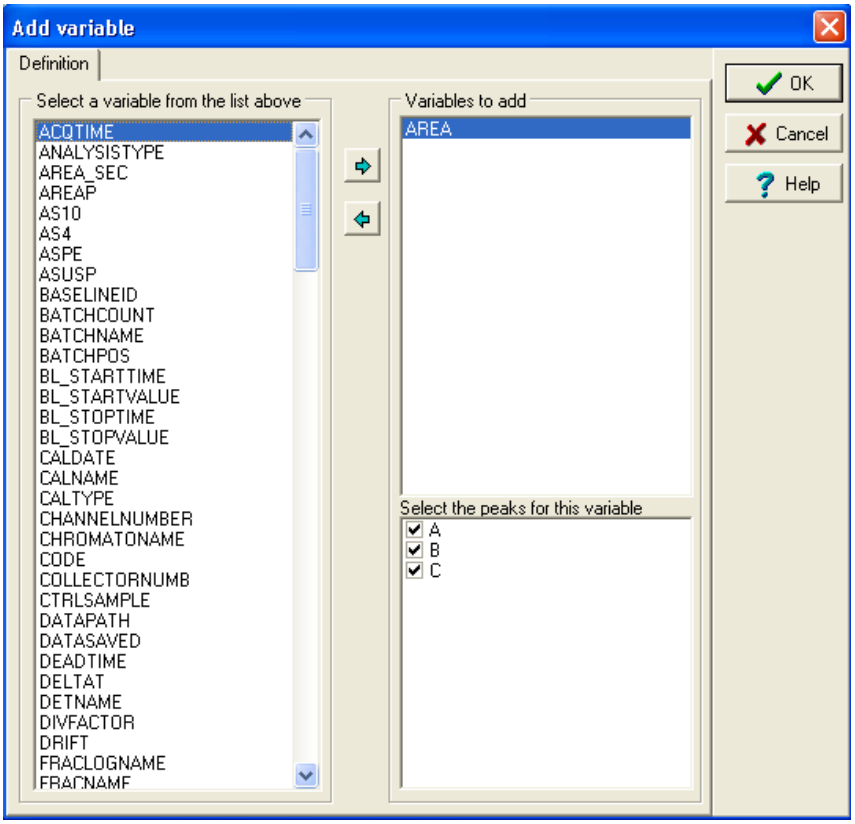


Choose the variables that will be added to the report. As the variables are defined in the method (custom variables and peak and group names), it is necessary to define a method name: Press the open ( ) icon and, in the Open file window, select the method corresponding to the type of sample to be added. This method contains the user-defined variables, as well as the names of the peaks (important if viewing a peak variable) and the format of the variables.

If the selected method contains several channels, user must specify in the following screen the channel of interest (only the variables and the peak names defined for this channel can be selected for the current summary report).



Then, in the variable list, press the left mouse button. Choose the ADD VARIABLE option. A window called ‘Add variable’ appears:

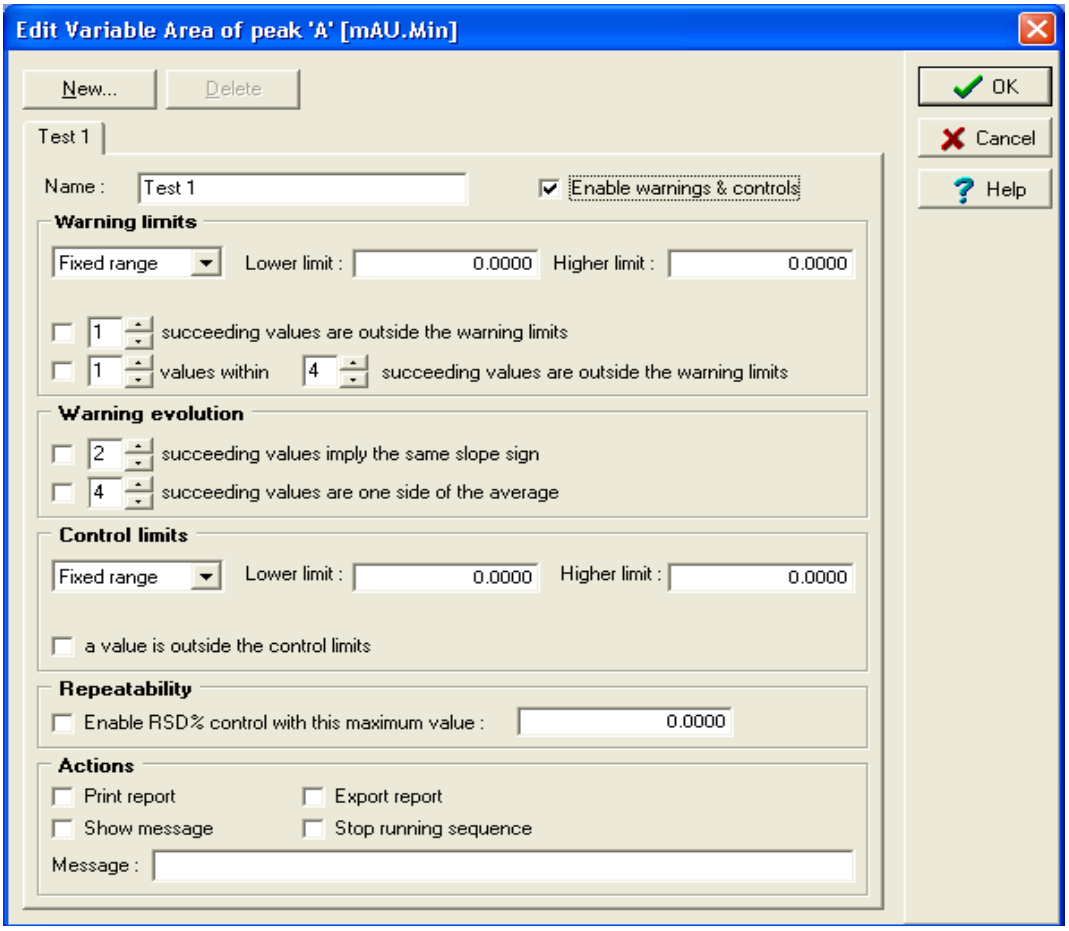


In this screen, select a variable to be added to the summary report. If the variable is a peak or a group variable, it is necessary to specify the peak(s) or group(s) concerned.

First select the name of the variable in the list, by double clicking on it or by using the arrow button. Then select the peaks concerned in the peak selection screen. By default all the existing peaks or groups are selected, the user can unselect some of them by unchecking the corresponding check box, or unselect or select all in a single action, thanks to the contextual menu.

Then validate by OK.

It is possible to define validity limits for variables added in the summary report. For that, select the variable in the ABC Variables screen, and press the button. The following screen is displayed:

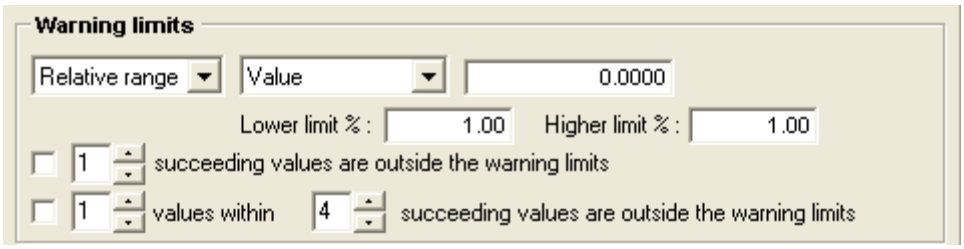


Check *Enable Warning & Control* to define limits for this variable. There are two kinds of limits: warning limits and control limits.

Warning limits are defined to advise that some problems could occur.

Control limits are limits that should never be overstepped.

Warning limits can be defined as: a fixed range, user has to define Lower and Higher limit, or as a Relative range in comparison of value, a variable or a variable mean.



Then define the conditions of the test:

- X succeeding values are outside the warning limits
- X values within Y succeeding values are outside the warning limits

User can define a Warning evolution:

- X succeeding values imply the same slope side
- X succeeding values are one side of the average

Control limits are defined in the same way as Warning limits, the same options are proposed.

Check the box Enable RSD% *control with this maximum value* and enter a value for the max %RSD.

When that option is chosen and when the %RSD is computed (see page 195), the software compares the %RSD computed for the variable to the max %RSD. A new warning is generated when the computed RSD is greater than the Max RSD%.

When the warning and controls are clearly defined, define the action to perform in the case or the test fails, among the four proposed:

Print a report, *Show message* (to define in the corresponding field), Export a report or in the case or the processed chromatogram is just acquired via a sequence, *Stop running sequence*.

It is possible to execute several tests on the same variable. For that, click on the

button. A new tab is added defining the new test conditions. You also can delete a test by activating the

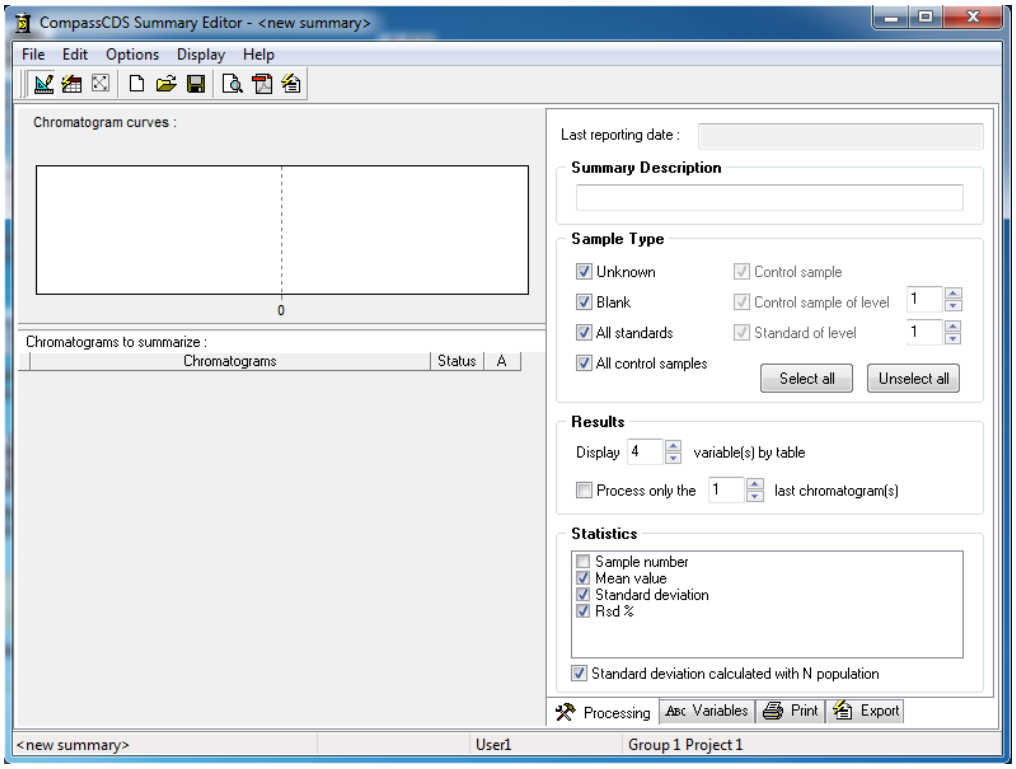
button.

When all tests are written for the selected variable, press OK. You can then select another variable and define tests.

If several variables are listed in the ABC Variable tab, you can sort them by using the up and down buttons: and , it can be useful to group all the variable of same type in the same result graphic.

Report

Select the Print tab; choose what should be printed and when the report should be printed.



First, enter a report header. This header will be printed at the top of the first page of the report.

In the Report options zone, choose what should be printed

Comments: the comments entered in the bottom of this screen,

Tables: to print the tables containing the variable values for each chromatogram,

Curves: the graphical evolution of the values,

Chromatogram list: the list of the chromatograms with their acquisition date,

Event log: the summary of all the processes done in the summary,

Warnings: the warning if some variable exceeds the limits defined in the Add variable screen,

Variable list: the list of the selected variables

Section titles: titles for all the previously selected items.

Then, in the Print report on zone, choose when the report should be printed:

At the end of every sequence or reprocessing list or at the end of every single acquisition (launched with the Quick Start).

NOTE: Report can also be printed after a warning or a control exceeding, but the print action is then defined in the variable's warning and control screen.

Note that if several summary reports are defined in different lines of the sequence or of the reprocessing list and that you have selected Sequence completed or Repro.list completed, only the summaries defined in the last line of the sequence or of the reprocessing list will be printed. To print automatically a summary report after reprocessing , select the option Repro.list completed.

NOTE: An index is associated to each chromatogram name, and this index is displayed in the array giving the statistical results instead of the entire name:

Chromatogram List

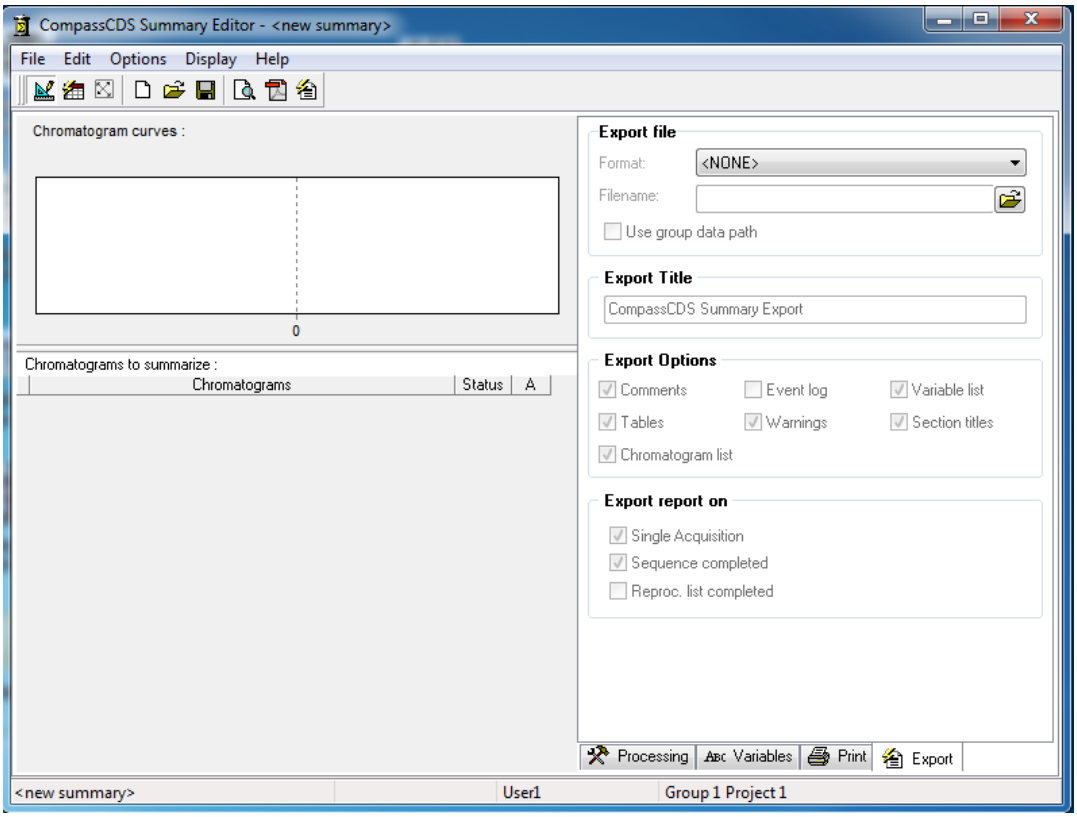
#1 - 2P-101.DATA [Channel 1]
#2 - 2P-102.DATA [Channel 1]
#3 - 2P-103.DATA [Channel 1]

Array 1

	Area/compound 1	Area/compound 2	Area/compound 3
#1			12100,1
#2			20558,4
#3			20537,0
Mean	0,0	0,0	17731,8
Std Dev (n)	0,0	0,0	3982,2
Rsd %	0,00	0,00	22,46

Export

Summary report can be automatically exported. Select the export tab.



In the Export File field, select the export file format (Excel, Word…), and specify data path and file name.

In the Export Title field, define a file name that will be displayed in the exported summary report.

In the Export options part, select which part of the report should be exported.

In the Export report on part, define when the report should be exported: at the end of the acquisition, the sequence or the reprocessing list.

Once export options have been set, save the summary.

Summary reports can be manually exported according to what has been defined in the "Export" tab, click on to do so.

How to Add Chromatograms in the Summary Report

Inside the Summary Editor:

To add chromatograms in the summary editor, select the FILE / OPEN / OPEN SUMMARY REPORT menu. In the Open file window, select the summary report to which chromatograms will be added. The summary report is opened in CompassCDS summary editor.

In the summary editor, press the right mouse button inside the panel called ‘Chromatograms to summarize’. Of course, if some chromatograms have already been added to the summary, they are listed in this zone. In the popup menu, choose ADD CHROMATOGRAM. It is also possible to use the main menu and select EDIT / ADD CHROMATOGRAM. Select the chromatograms and the channel to summarize in the Open file window and press OK.

The chromatograms are added to the summary, press the Results mode button to view the statistical results.

Automatically:

A chromatogram can be added automatically during processing in CompassCDS, after a single acquisition, after an acquisition in a sequence, or after the reprocessing of the chromatogram. In the method used to process the chromatogram, select the name of the summary report to which it should be added.

NOTE: It is possible to choose to add only a few chromatograms processed with the same method (in which a summary report is defined) in the summary report. If a chromatogram is processed and does not need to be added to the summary, uncheck the summary report options in the Processing page (see page 194).

Chromatograms Management in the Summary Report:

In the Summary Report, there is a list of the chromatograms that have been summarized (added to the summary).

These chromatograms are annotated:

	This symbol means that all the variables defined have been found in the chromatogram.
	This symbol means that a variable is missing in the chromatogram
	This symbol means that the chromatogram has not been found.

Additional information about the chromatogram is available by selecting CHROMATOGRAM INFO from the popup menu (by clicking the right mouse button) of the chromatogram list.

The popup menu helps to manage the chromatogram list. Most options are also available in the EDIT menu:

Add chromatogram: Use this menu to manually add chromatograms to the summary report.

Delete chromatogram: Use this option to remove the chromatogram from the summary report

Delete all: Use this option to remove all the chromatograms from the summary report.

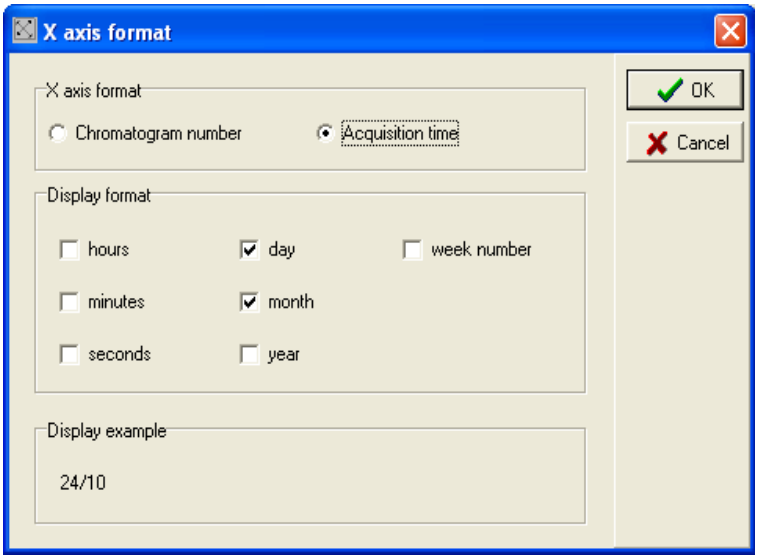
Chromatogram info: View the information about the chromatogram.

It is possible to deactivate a chromatogram for a period: its results will not be considered in the statistics. Uncheck the cell in the 'A' column: check it again to reactivate it.

Editing the Summary Report Results:

To view the summary results, press the Results Mode icon.

The tables summarizing the variable values are displayed with the corresponding graphs. To customize the X axis format, select the icon, the following screen is displayed:



By default the chromatogram number is displayed on the X axis of the graph, but the user can choose to display acquisition time and configure the time format to display.

To print the report, press the Print report icon . A preview of the report is displayed, and then presses the *Print button*. To print the report as pdf, press the Print as PDF icon:

Importing a Chromatogram (AIA format)

To import a chromatogram, copy it to the working folder and open it with the open file window as a chromatogram acquired with CompassCDS.

The chromatograms available in an AIA format are displayed as CompassCDS chromatograms in the open file window, except that their extension is .cdf instead of .data. They also contain no information or preview, and the control and acquisition sections of the method are missing.

When an imported chromatogram is opened in CompassCDS, it is displayed with CompassCDS integration and the results are calculated according to CompassCDS integration events. The peak identification parameters are not kept. Some variables concerning the acquisition are also imported: acquisition date, channel number, chromatogram name, operator name, etc.

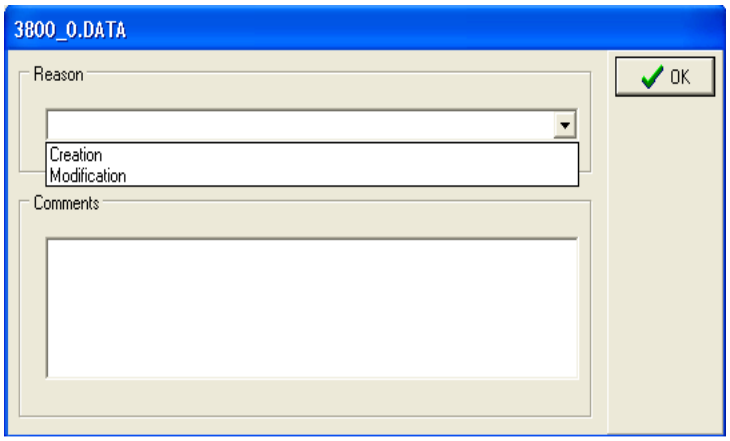
When the chromatogram is saved in CompassCDS format, a .DATA file is created.

Audit Trail

The audit trail is a tool used to trace the history of a file. Each time a chromatogram, a method, a calibration curve, a sequence, etc. is modified and saved, an archive is generated. This archive describes all the changes made, specifies the name of the user that made the change, when the change was made, and it also gives the reason and comments for change if entered by the user at the time of saving.

The audit trail is tracked only if the corresponding option is set in the profile associated with each user (CompassCDS Configuration Manager). All files or, only a few ones can have an audit trail. It must be configured in the “Audit Trail” profile.

CompassCDS offers the possibility to define or not a reason and eventually a comment for the change. If this option is selected in the CompassCDS Configuration Manager, when saving a file the following box is displayed:



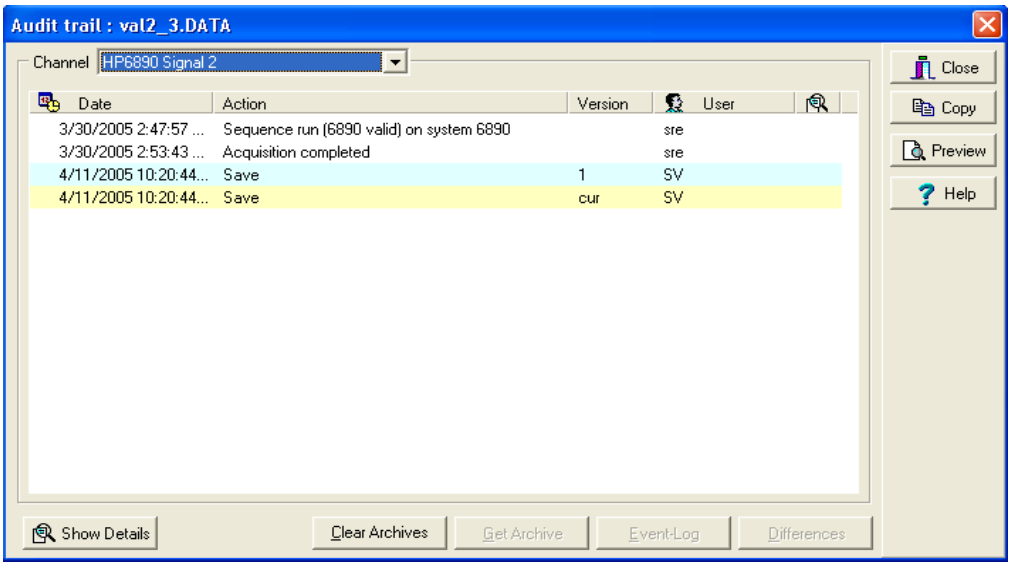
The user has to select a reason in the list given in the scrolling bar (the list is captured from the CompassCDS Configuration Manager: “Policies\Audit Trail\Configure reasons\CompassCDS

changes menu). If a mandatory comment must be entered and this is not done, then the user cannot validate and the following message appears on the screen:

The validation is possible only when a comment is entered.

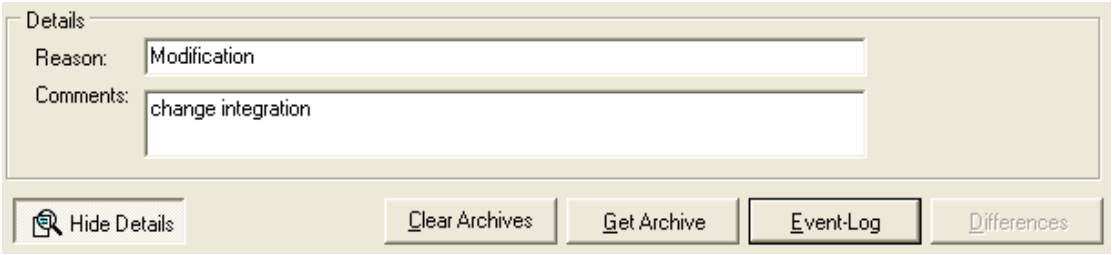
To view the audit trail of a file, open-it, then select the DISPLAY / AUDIT TRAIL menu, the AUDIT TRAIL popup menu or press the icon.

In the case of a chromatogram, the following screen is displayed:



The *audit trail* of a chromatogram or of a method are the same: Show details, Clear archives, Get archive, Event Log buttons are proposed according to the profile of the user.

This button allows the reason to be viewed and any comments entered at file saving to be viewed. Reason and comments are not mandatory, it is an optional function defined in the profiles (CompassCDS Configuration Manager). Clicking on it causes the following box to be displayed:



Clear Archives This button allows the user to clear the archives for the file. When this action is achieved a line appears in the audit trail, mentioning the operation. This button is displayed only for a user having the corresponding profile (CompassCDS Configuration Manager).

Get Archive This button allows the user to recover an old version of the file. It is, for example, possible to recover an old version of a method to process chromatograms or to use an old calibration curve version to quantify chromatograms.

Event-Log This button allows the user to view in detail the operations made. For example, each step of the treatment of a chromatogram: pre-processing, integration, identification, etc...

Differences This button is active only if two versions of the file, consecutive or not, are selected. It quickly shows the differences between the two selected versions.

NOTE: In the case of a calibration curve, the two selected versions must belong to the same calibration curve that means that two versions made before and after a “clear old points” could not be matched.

Close This button allows you to quit the Audit Trail.

Copy This button allows you to copy the Audit Trail to another application.

Preview This button allows you to view the audit trail report before printing.

Help This button allows you to reach the “On line help” (Internet Explorer has to be installed on the computer).

Save as... This button is available only if the "archive calibration curve" profile has been selected in the CompassCDS Configuration Manager. Archives are saved as calibration curve and can be used for chromatogram processing.

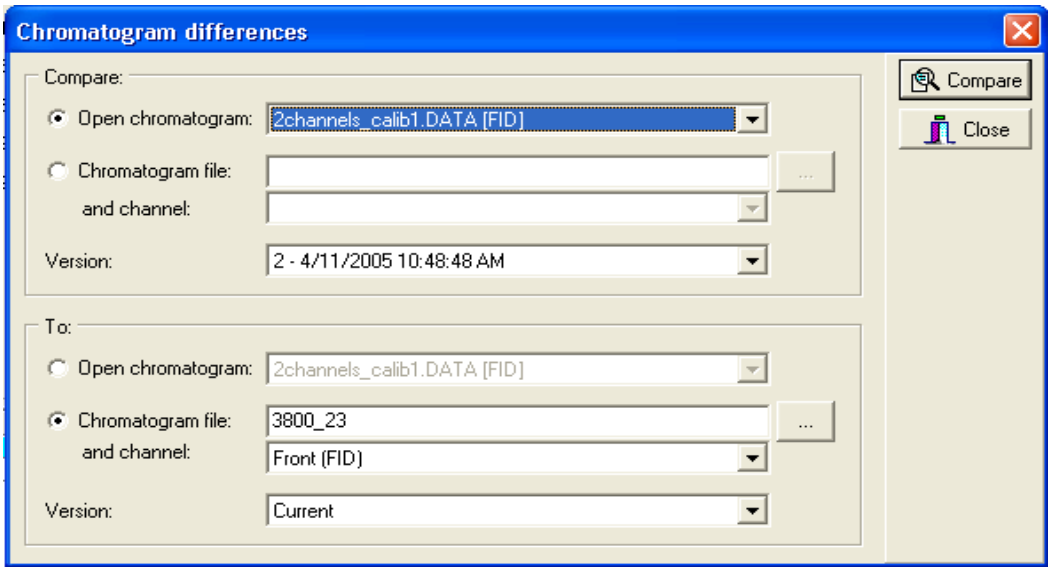
Note that for a calibration curve, the Event Log button is absent and a Save as button is present.

In the case of sequences and reprocessing lists, only the Show details, Clear archives, Get archive, and Event Log buttons are present. It is impossible to get an old version of such a file or display differences between two versions. In fact, no archives are created for these files, only a list of changes is created. Therefore, archive sequence and archive reprocessing list profile do not exist in the CompassCDS Configuration Manager.

How to Compare Two Chromatograms

CompassCDS allows you to quickly compare two chromatograms, or two archives of the same chromatogram, if the archive option was defined in the profiles in the CompassCDS Configuration Manager (“Audit Trail Profile”). The chromatograms to be compared need not necessarily to be opened.

Select the DATA / CHROMATOGRAM DIFFERENCES menu, the following screen appears.

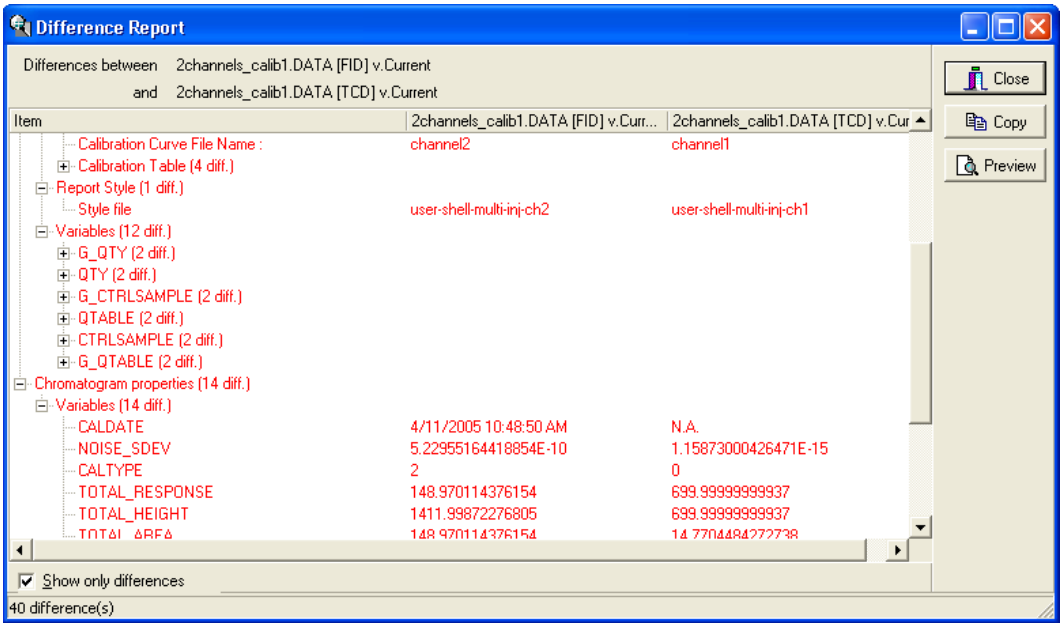


The two chromatograms to be compared are defined in the two sections of the screen.

If a chromatogram is opened and selected, its name is displayed by default in the “Open chromatogram” box. To compare a non-opened chromatogram, select its name in the “Chromatogram file” field. Define the channel to be compared in the corresponding field. In the “Version” field, select the chromatogram version to be compared, in the case where the archive profile is defined.

Once both chromatograms to be compared are defined, click on the Compare button, the differences are then displayed.

Differences only are listed if the “Show only differences” option is checked, or detailed if not. Only the differences for the chromatogram method are displayed:



User can print the difference by clicking on the

button, then on the button in the previous screen. He can also copy the differences to paste them in another application.

Electronic Signature

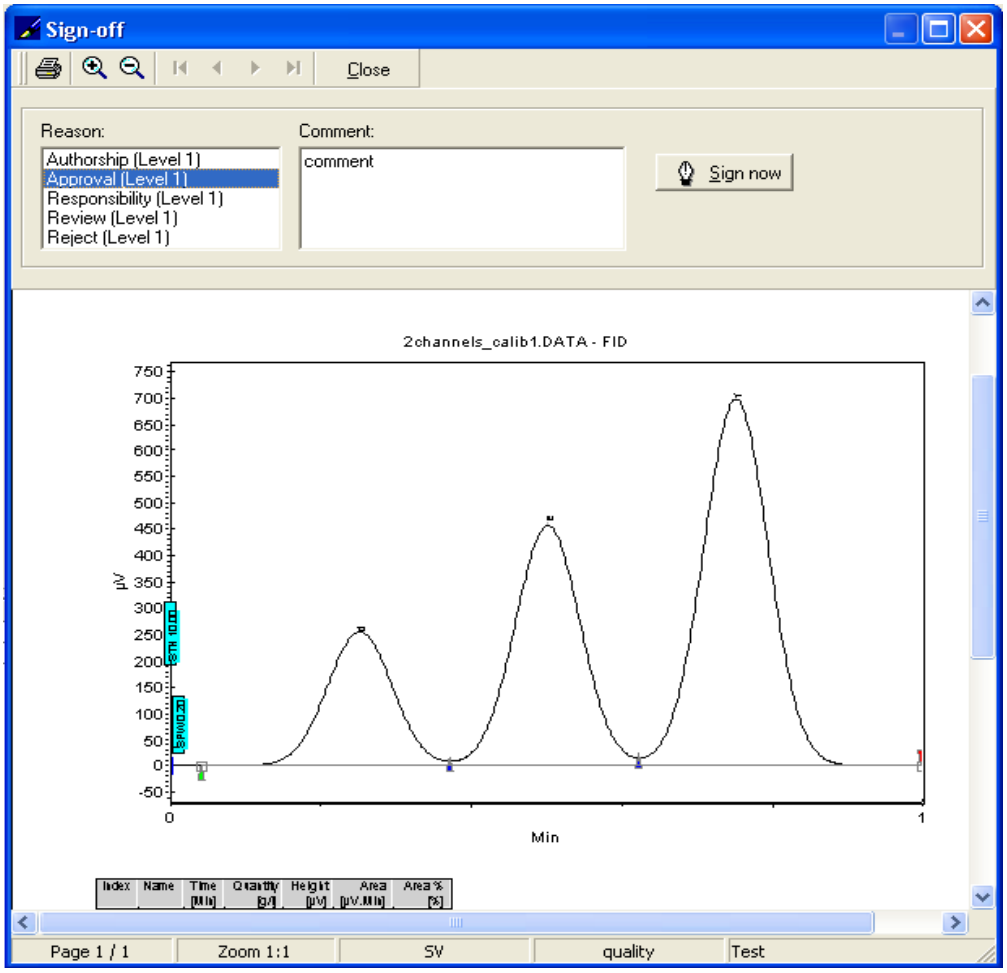
To satisfy the regulatory requirements of the FDA 21CFR11 (“rule 11”), CompassCDS offers the capability to electronically sign one or several data set for validation. Signing is executed within CompassCDS and the signature can also be printed if declared in the CompassCDS Report Editor (printing manager).

The electronic signature is accessible from CompassCDS. User can sign a single chromatogram or a batch of chromatograms.

Single Chromatogram Sign Off

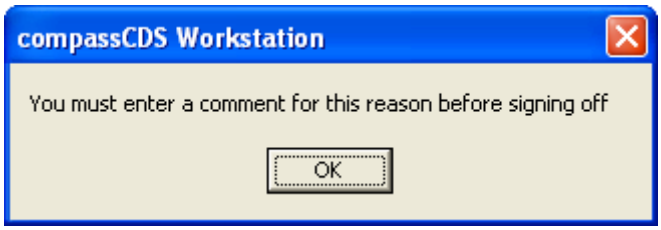
The chromatogram to be signed must be open and a report style must be associated with the chromatogram.

Click on the icon and the following screen is displayed:

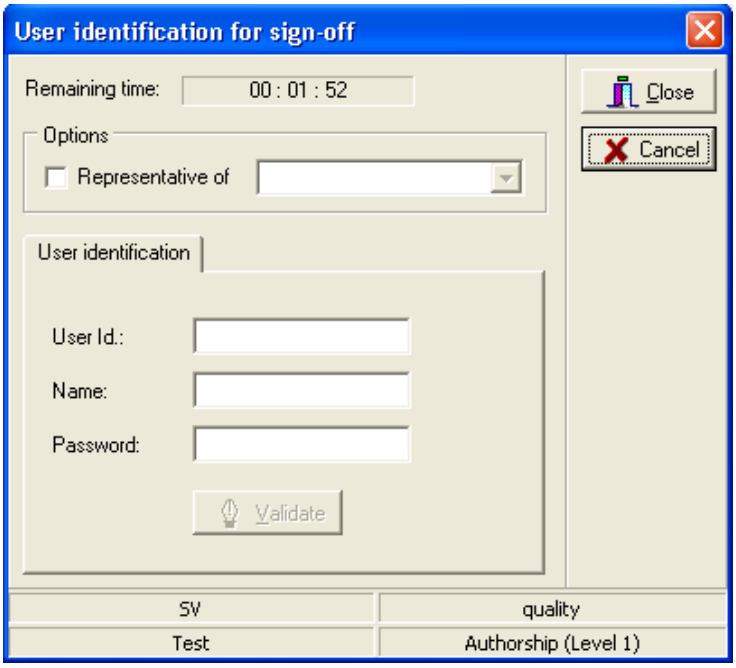


If several pages are defined, then the user has to view all the pages of the report in order to be able to sign. He must then define a reason and possibly a comment, once this is done, he can click on the button to open the sign off box.

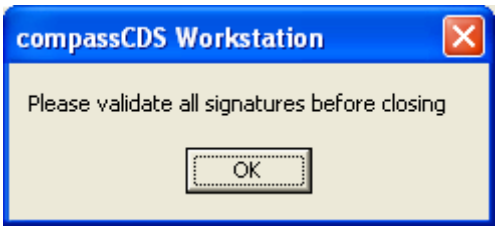
If no comment has been entered when it is mandatory, the following warning message will appear:



The following sign off window is displayed:

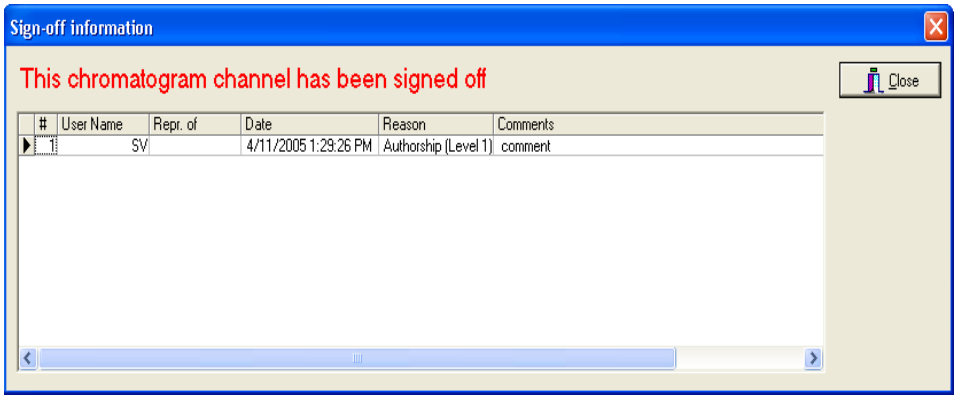


To sign, a user must identify the User Id / Password combination (defined in the CompassCDS Configuration Manager) is unique in order to formally identify the signatory. A password must have been defined; otherwise it is not possible to sign off. The user must sign within the delay defined in the CompassCDS Configuration Manager, via the POLICIES / CONFIGURATION / ELECTRONIC SIGNATURE menu (from 2 up to 10 minutes); a counter shows the remaining time and once the delay time has elapsed, the screen will close. If the user identifies within the delay period, the Validate button is active. This button must be pressed to sign off otherwise the following message will appear when closing the screen:



Several users can sign as representatives of a missing signatory. The number of representatives can be defined in the CompassCDS Configuration Manager (POLICIES / CONFIGURATION / ELECTRONIC SIGNATURE menu): at least two different users can sign as representatives of a missing one. All the representatives must also sign within the delay defined in the CompassCDS Configuration Manager, while the Validate button is active. The name of the missing signatory is selected from the list in the scrolling bar, where the names of all users defined in the project is shown.

To view the sign off for a file, open it and then click on the icon. The following screen is displayed:


Sign-off information
This chromatogram channel has been signed off
Close
User Name Repr. of Date Reason Comments
1 SV 4/11/2005 1:29:26 PM Authorship (Level 1) comment

The name of the signatory, if applicable the name of the representative signatory, the date of the sign off, the reason and any comments are displayed.

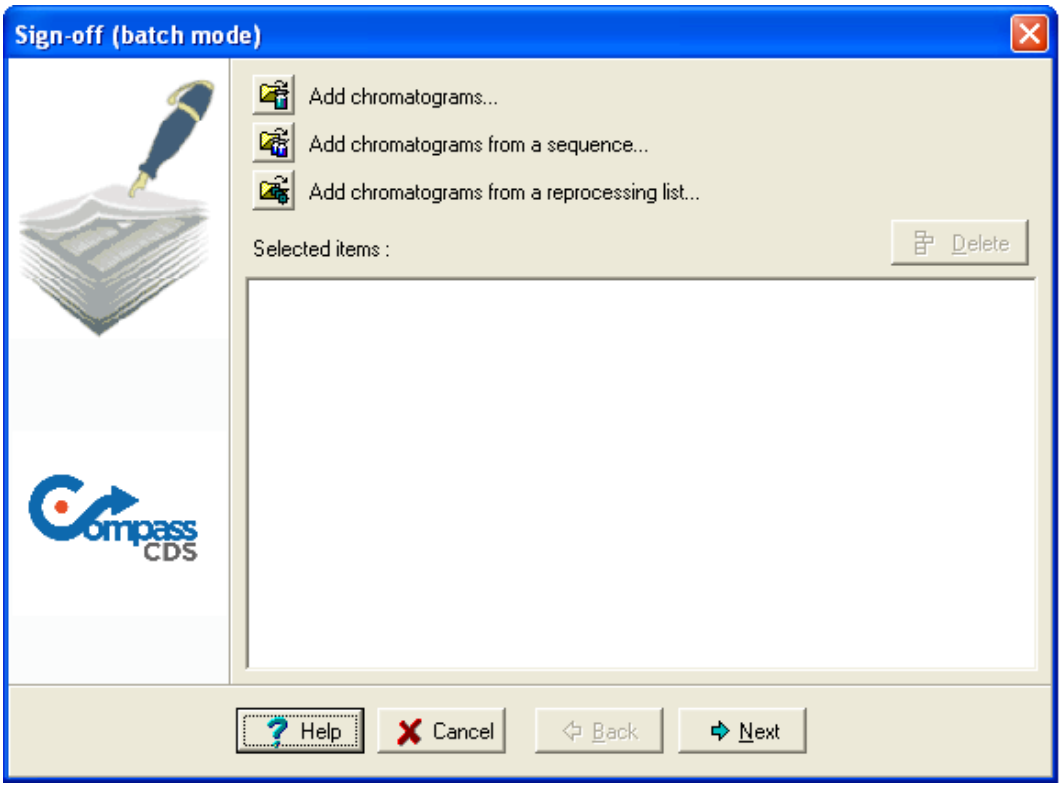
NOTE: If a change is made to the chromatogram file (integration, identification, quantification, etc.) and saved after the sign off, the sign off is deleted and must be repeated if necessary.

Chromatogram Batch Sign Off

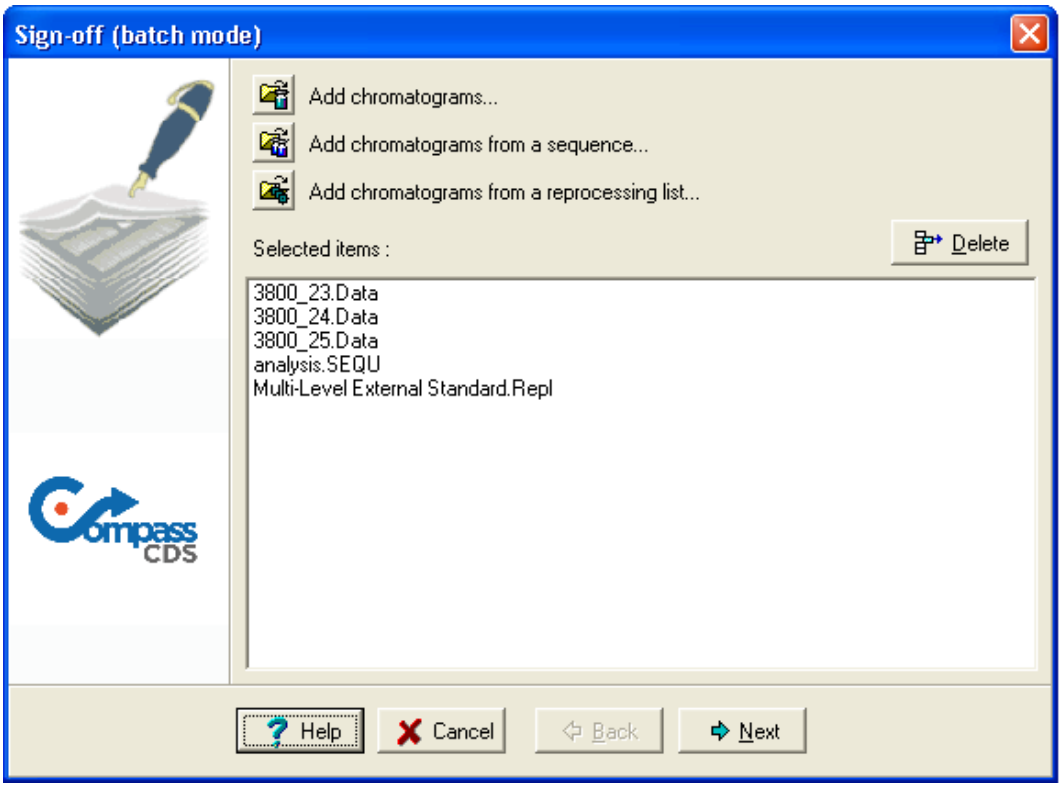
Signature of chromatograms one by one

An option allows the user to sign several chromatograms in batch. A report must be associated to each chromatogram.

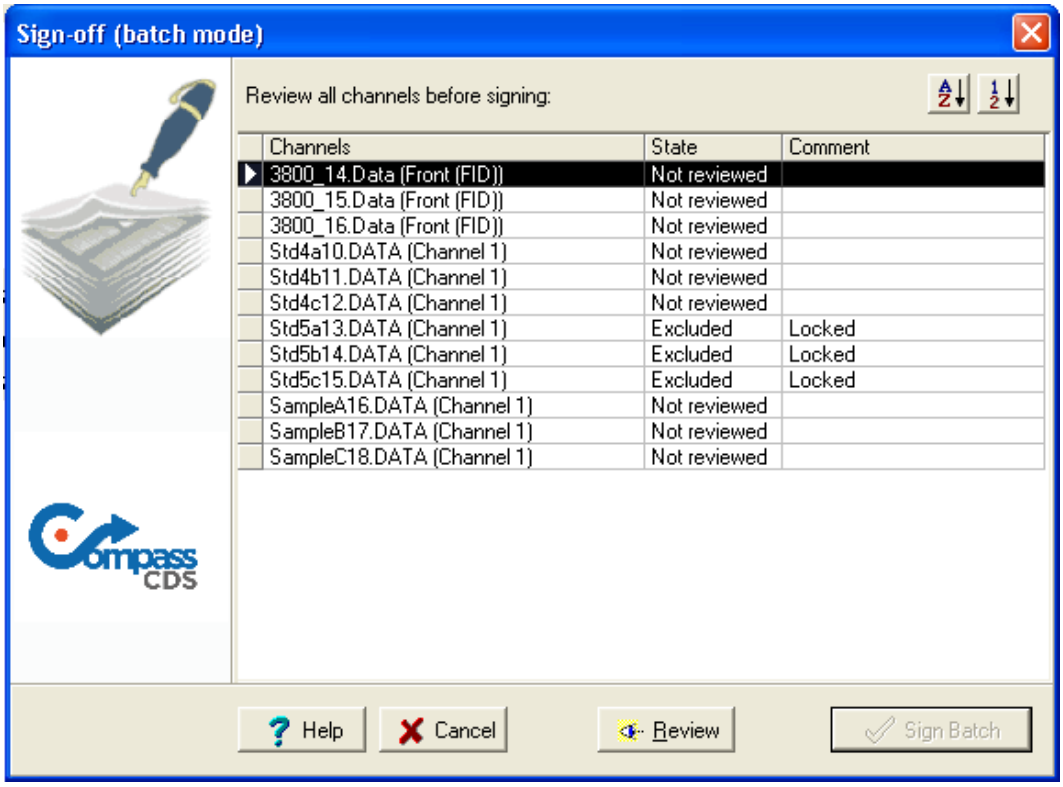
Select the icon. The following screen is displayed:



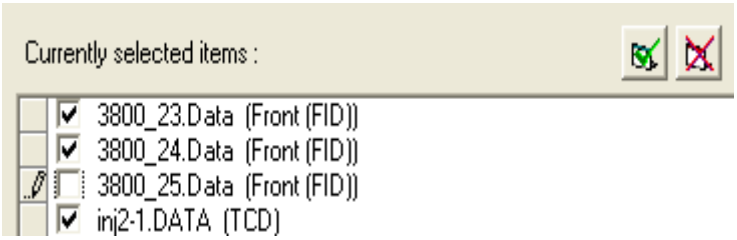
User can add chromatograms by selecting the Add chromatograms option, or all the chromatograms acquired within a sequence by selecting the Add chromatograms from a sequence, or all the chromatograms contained in a reprocessing list by selecting the Add chromatograms from a reprocessing list. The selected objects (chromatograms, sequences or reprocessing lists) are then listed in the Selected items field.



Then click on NEXT. The screen listing the chromatograms to sign is displayed:



The chromatograms corresponding to the previous selection are listed in this screen, one line is added by channel. The user can remove some chromatograms from the list by un-checking the associated box. To check or uncheck several chromatograms in a single action, you can use the Shift and Ctrl keys, or extend the selection of the lines:

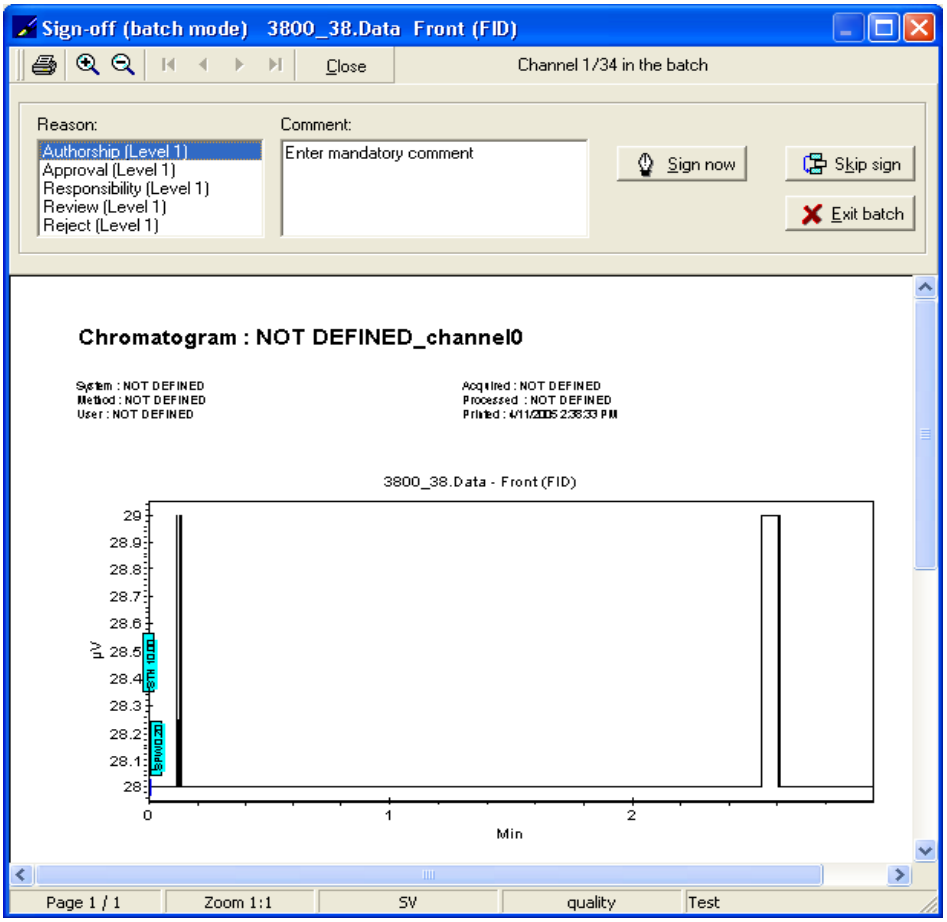


Then click on the Check selection icon or Uncheck selection icon .

It is also possible to sort the chromatograms either by name ( ) or by channel ( ), to make the selection easier.

Once the chromatograms to sign have been selected, click on the Begin review button.

The following screen is displayed:



The report of the first selected chromatogram is displayed. The user must read all the pages of the report to be authorized to sign it. If a mandatory comment is required, the user must enter it in the corresponding field before pressing the button.

A message indicates in the top of the screen, the position of the current chromatogram in the batch: means that the user signs the first chromatogram on a list of height.

If pressing the button, the following screen is displayed:

The user must enter his User Id and password in the corresponding fields, click on Validate to confirm the signature, then on the Close button to exit this screen.

NOTE: Some users can sign as representative of a user, as in the single chromatogram process (see p 62). In that case, all the representative users must sign each chromatogram together.

The screen displaying the report of the following chromatogram is then displayed; the user must read the report in total, and then press the Sign now button. The same screen as the previous one is displayed again, but the User Id is pre-defined, to avoid the user to enter it again. The user has to just enter his password for identification, and then validate the signature.

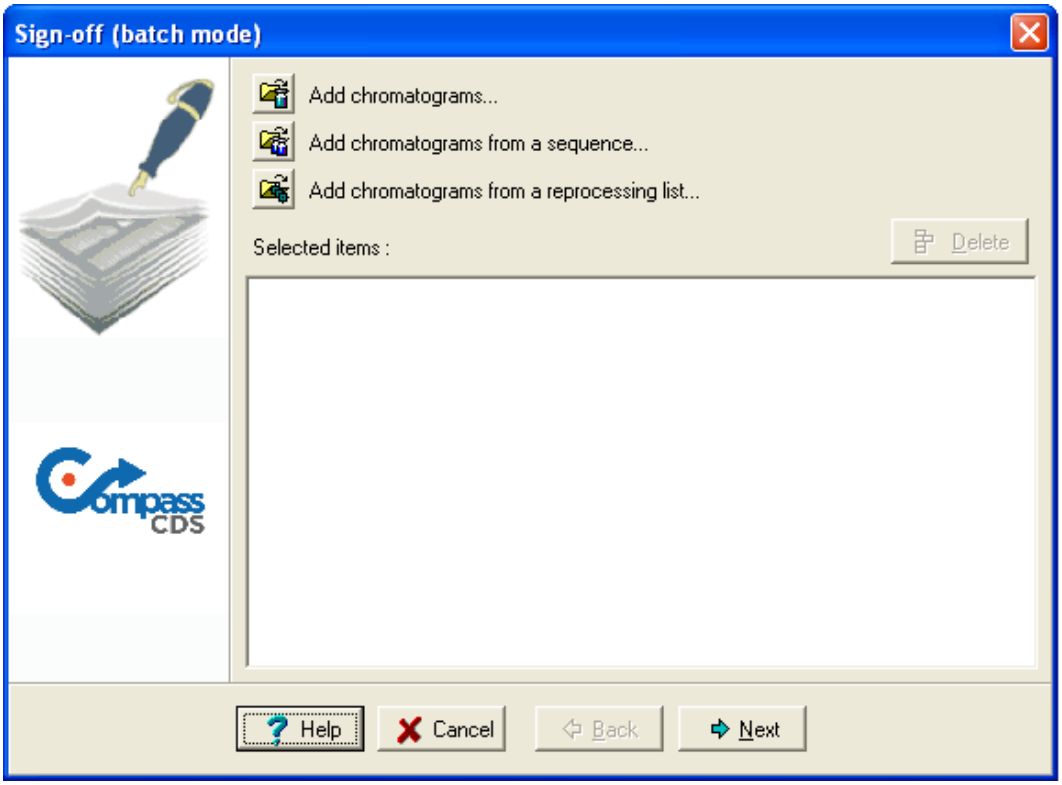
The operation has to be reproduced for each chromatogram to sign.

If the user does not want to sign one of the selected chromatogram, he can cancel the signature by pressing the Skip sign button in the report edition screen. The following chromatogram of the list is then proposed for signature. To stop the batch sign off process, press the Exit batch button, the batch sign of wizard is closed, the chromatogram selection is lost. In that case, all the already signed chromatograms keep their signature.

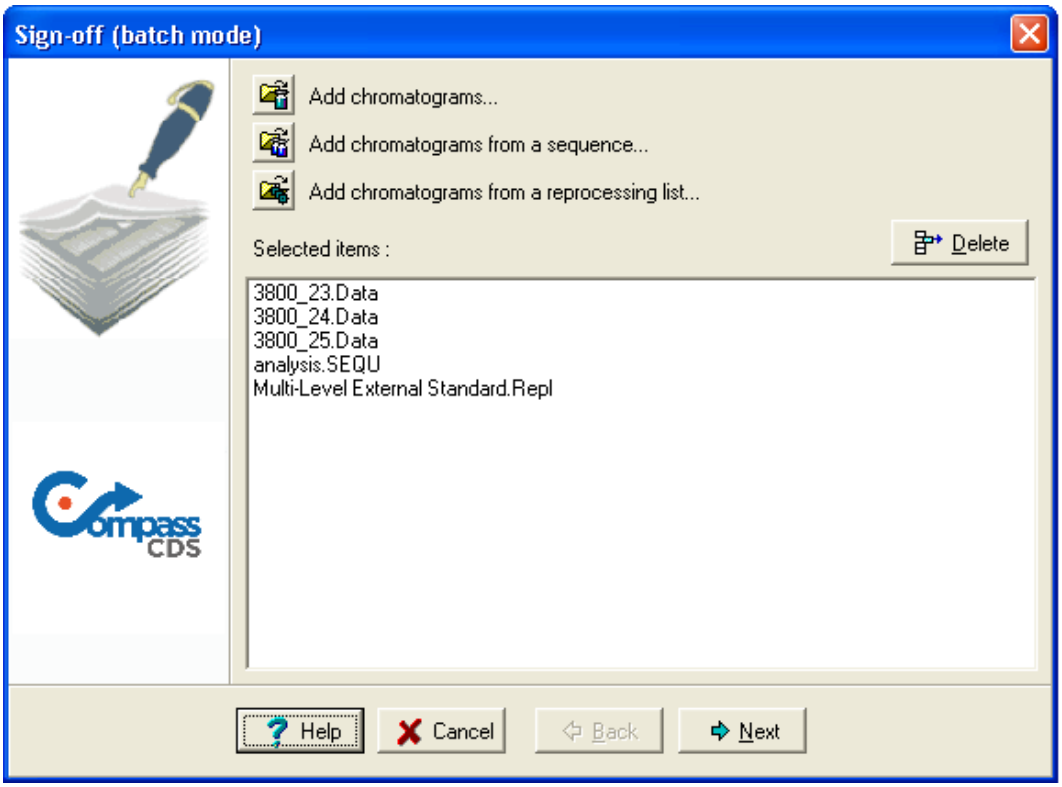
Signature of Chromatograms in One Batch

CompassCDS proposes an option allowing the user to sign several chromatograms in one batch, by defining only a single time its name, password, reason and comments. To use this function, the connected user must be assigned the '21CFR11-user / Electronic signature / Allow batch sign at once' right in the CompassCDS Configuration manager.

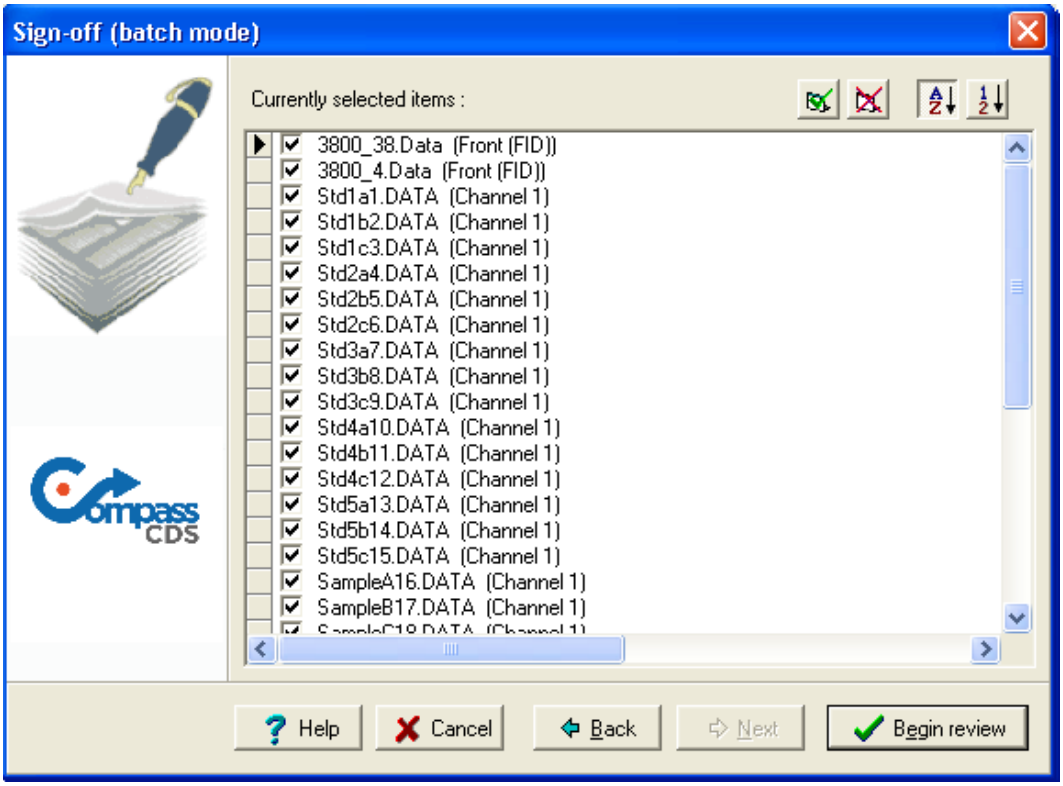
The user has to select the chromatograms he wants to sign in one batch by selecting the icon. The following screen is displayed:



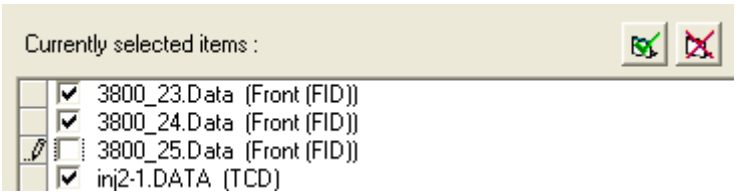
User can add chromatograms by selecting the Add chromatograms option, or all the chromatograms acquired within a sequence by selecting the Add chromatograms from a sequence, or all the chromatograms contained in a reprocessing list by selecting the Add chromatograms from a reprocessing list. The selected objects (chromatograms, sequences or reprocessing lists) are then listed in the Selected items field.



Then click on NEXT. The screen, listing the chromatograms to sign is displayed:

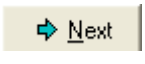


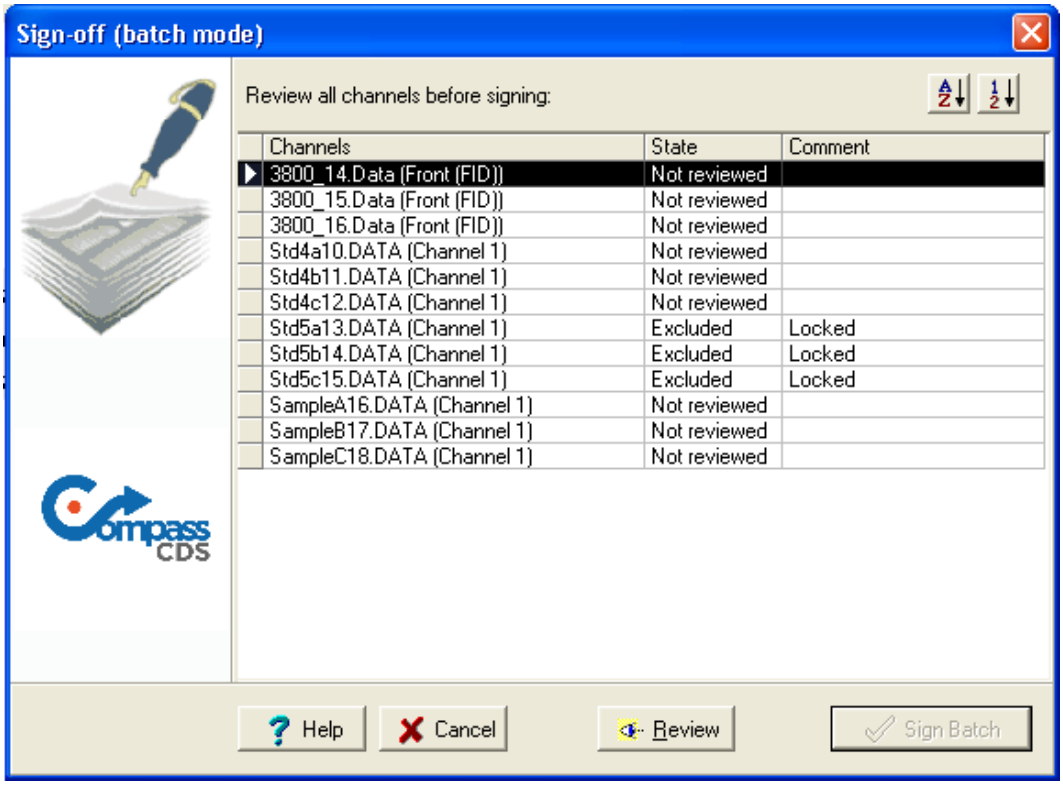
The chromatograms corresponding to the previous selection are listed in this screen; one line is added by channel. The user can remove some chromatograms from the list by unchecking the associated box. To check or uncheck several chromatograms in a single action, you can use the Shift and Ctrl keys, or extend the selection of the lines:



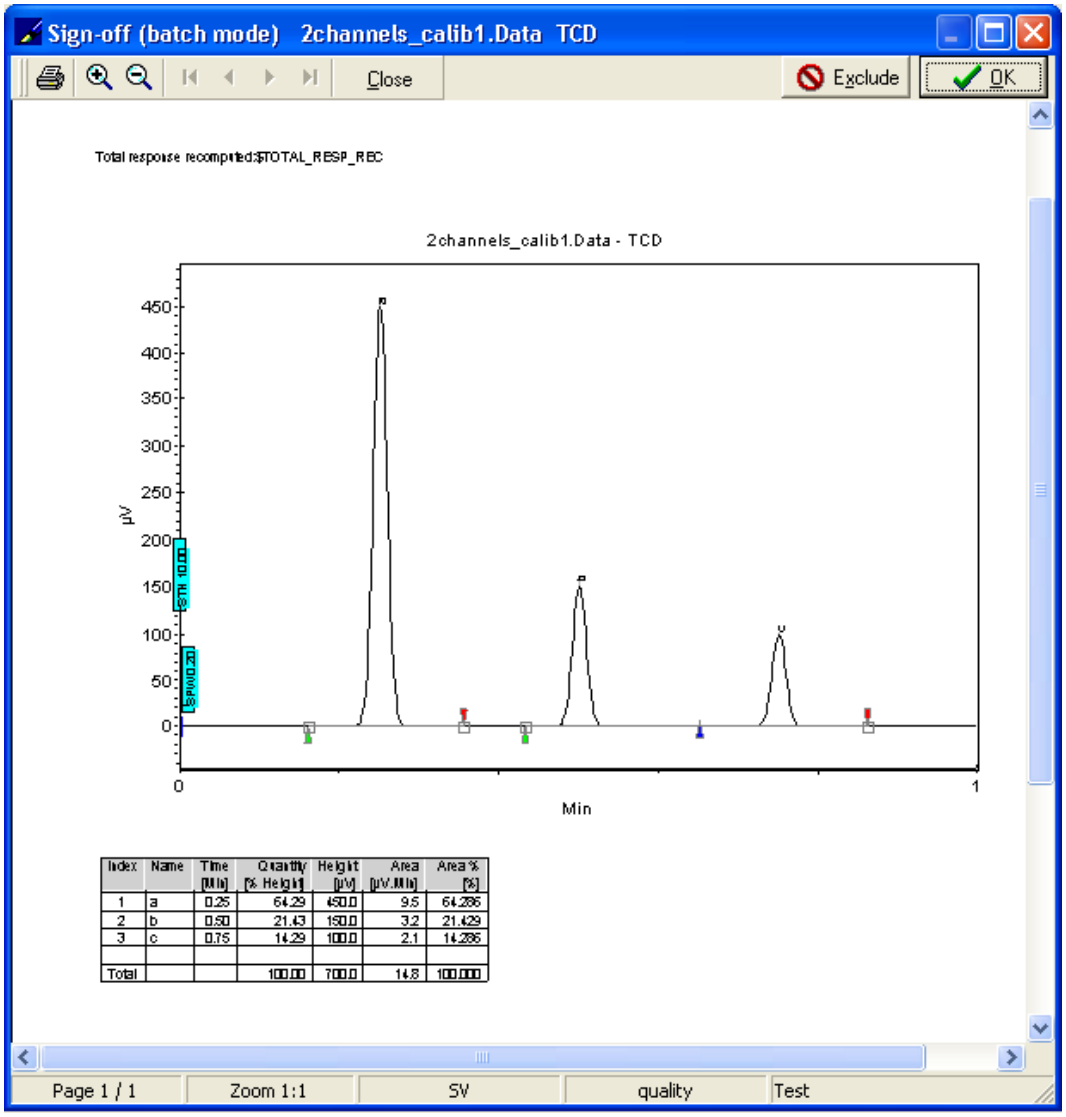
Then click on the Check selection icon or Uncheck selection icon .

It is also possible to sort the chromatograms either by name ( ) or by channel ( ), to make the selection easier.

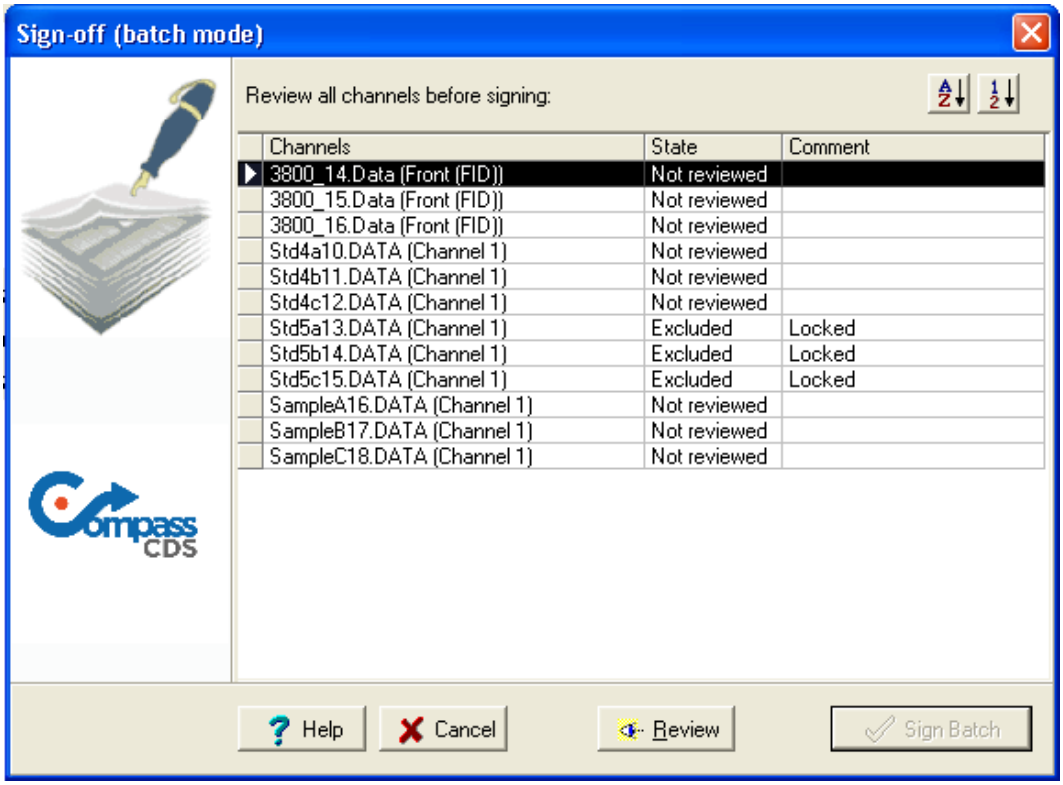
Once the chromatograms to sign have been selected, click on the  button. The following screen is displayed:



Click on the button to display the report of the first listed chromatogram.



Click on OK to accept to sign this chromatogram or on Exclude to exclude it from the batch of chromatograms to sign. Then the previous screen is displayed to show the signature progression:

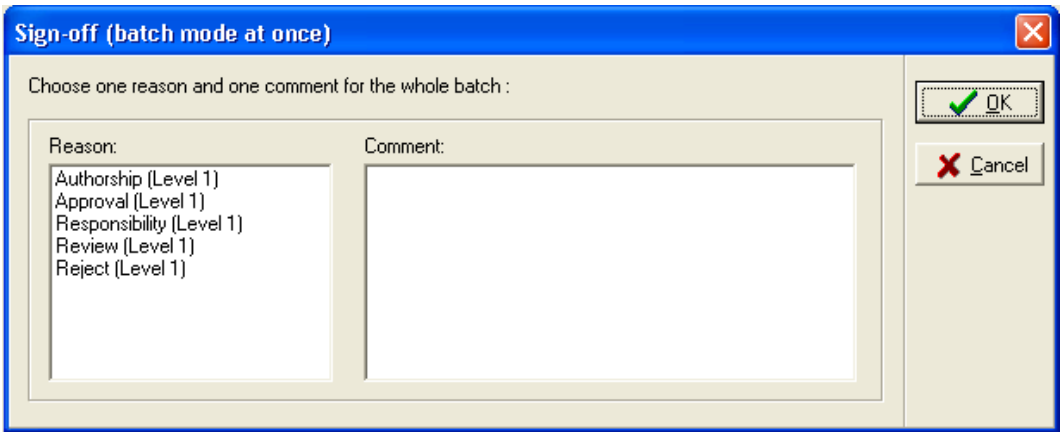


In case the user has 'Excluded' the chromatogram, 'rejected by user' is listed in the Comment column.

User has to select the

button until he has accepted or excluded all the listed chromatograms. Then the

button becomes available. By clicking on it, the following screen is displayed:

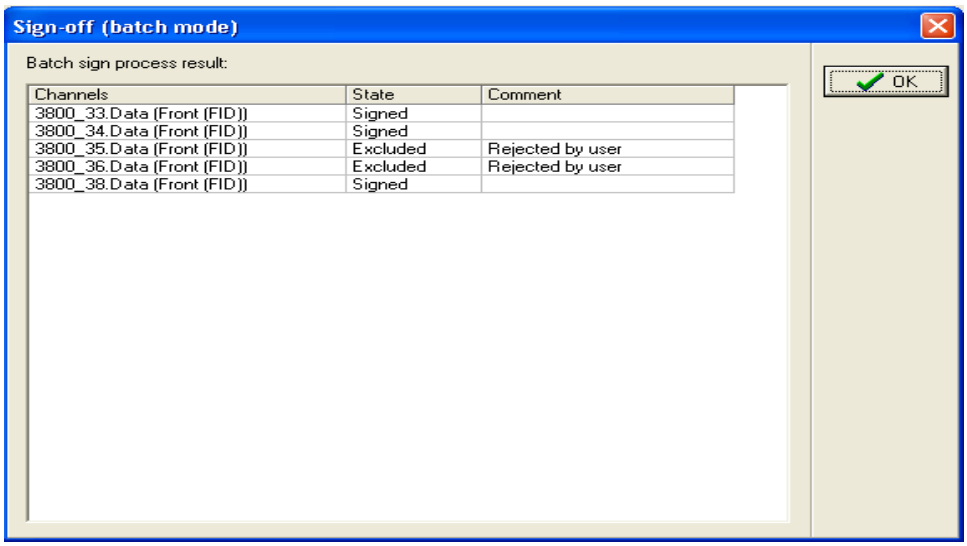


In this screen, the user selects the signature reasons wanted to assign to all chromatograms and optionally comments. Click on OK to perform the signature.

The user must enter the User Id and password in the corresponding fields, click on Validate to confirm the signature, then click on the Close button to exit this screen.

NOTE: Some users can sign as representative of a user, as in the single chromatogram process (see p 62). In that case, all the representative users must sign together.

The following screen is displayed to indicate whose chromatograms have been signed in the list.

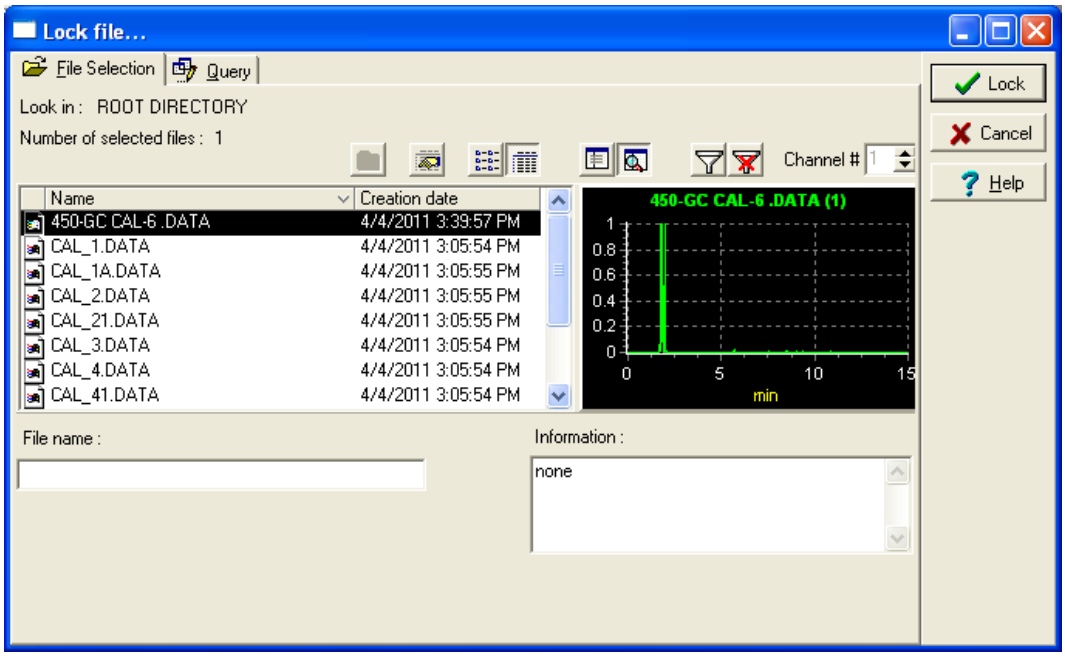


Lock/Unlock Chromatograms

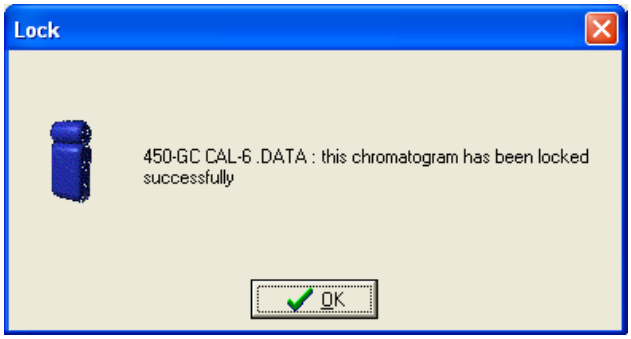
CompassCDS offers the possibility to lock (and then unlock) the chromatograms. A locked chromatogram can be open, printed, exported. A locked chromatogram can be modified but the modifications cannot be saved.

To lock one or several chromatograms, click on the icon or choose the FILE/LOCK CHROMATOGRAM menu.

The following screen appears:

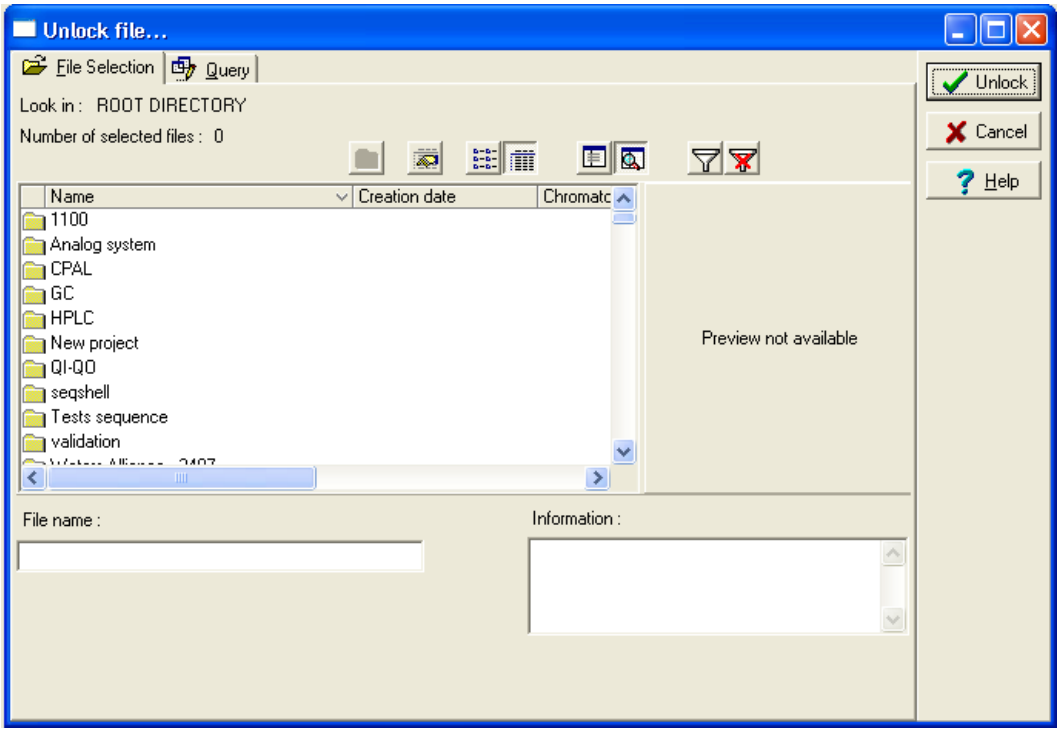


Choose the chromatograms to lock and click on the Lock button. A confirmation message appears as soon as the chromatograms are locked.

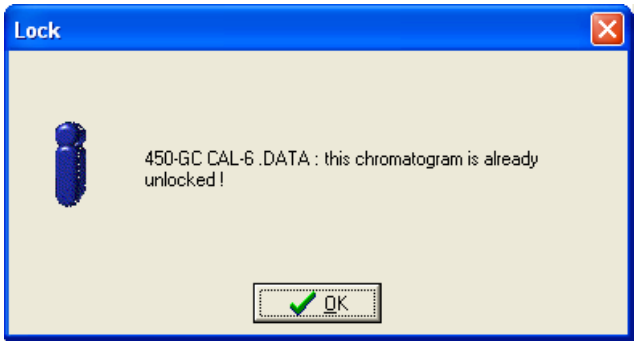


To unlock one or several chromatograms, click on the icon or choose the FILE/UNLOCK CHROMATOGRAM menu.

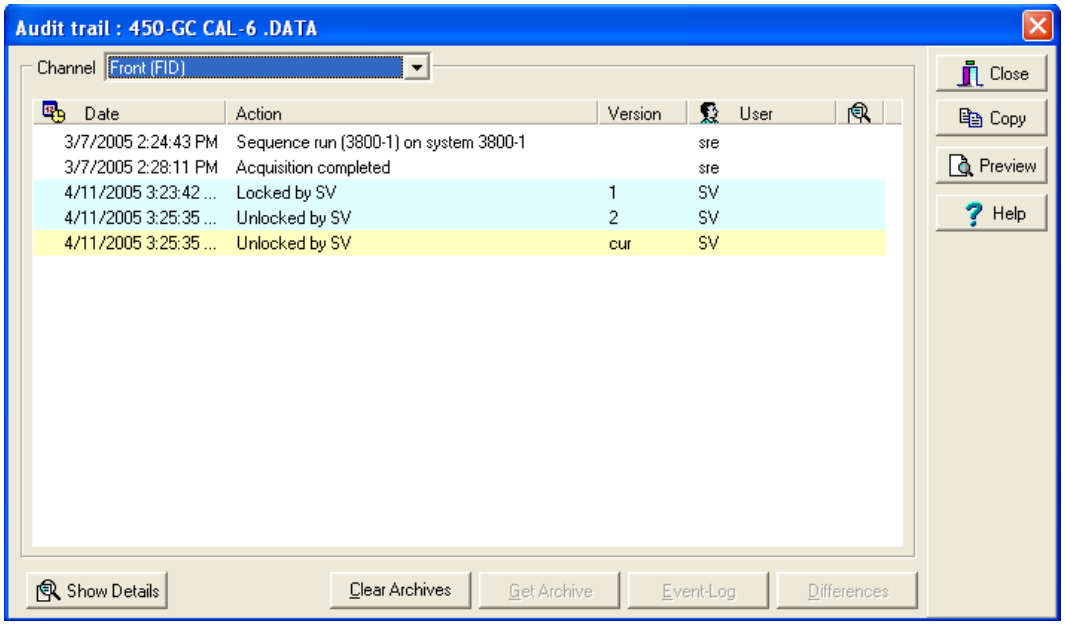
The following screen appears:



Choose the chromatograms to unlock and click on the Unlock button. A confirmation message appears as soon as the chromatograms are unlocked.



In the chromatogram audit trail, the lock and the unlock actions are listed as displayed in the following screen:


Audit trail : 450-GC CAL-6 .DATA
Channel
Front (FID)
Date
Action
Version
User
3/7/2005 2:24:43 PM
Sequence run (3800-1) on system 3800-1
sre
3/7/2005 2:28:11 PM
Acquisition completed
sre
4/11/2005 3:23:42 ...
Locked by SV
1
SV
4/11/2005 3:25:35 ...
Unlocked by SV
2
SV
4/11/2005 3:25:35 ...
Unlocked by SV
cur
SV
Close
Copy
Preview
Help
Show Details
Clear Archives
Get Archive
Event-Log
Differences

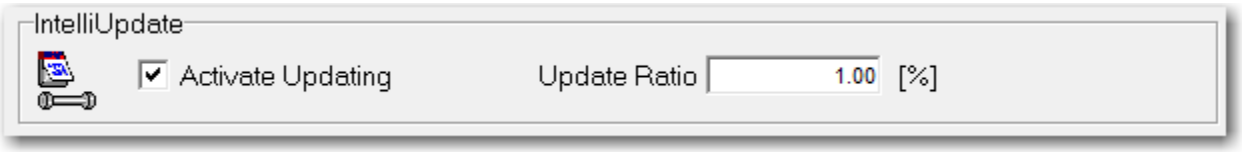
Advanced Parameters

This section concerns very particular applications used to answer specific user needs, and are not defined by default, during the software installation.

IntelliUpdate

CompassCDS contains an option enabling the user to simulate the ageing of a chromatographic column, by modifying automatically the theoretical peak and group retention times, as well as the integration event times in the method after an acquisition.

To activate this option, the user must be assigned a profile (CompassCDS Configuration Manager) containing the IntelliUpdate option in the Method directory.



An added part, named IntelliUpdate appears in the acquisition part

The user checks the ‘Activate column Ageing’ box to activate the function, and enters in the Ratio box the shift percentage to apply during the new retention time calculation of peaks and groups and integration event times (details of the calculation are described in this section).

‘IntelliUpdate” is applied from one acquisition to another, that means that at the end of an acquisition with this option, the method is automatically modified, and new parameters will be used for the next acquisition with this method.

IntelliUpdate is applied only during acquisitions (Quick Start and sequence). If a chromatogram is reprocessed via the ‘Integrate’ (F5), ‘Reprocess’ (F6) function or via a reprocessing list, no change in the peak and group identification and in the integration event tables is made in this method.

Once the chromatogram has been acquired, the ‘IntelliUpdate” part of its method is no longer accessible, so it cannot be modified.

To apply calculation of ‘IntelliUpdate” the user is required to define reference peaks in the peak identification table. If no reference peak is defined, or if at least one of the reference peaks defined is not found in the chromatogram, the ‘IntelliUpdate calculations will not be done.

Calculation details:

For all the peaks defined in the identification table and present in the chromatogram, the time limit of groups and the integration events time, the following calculation is applied:

$$RT'_{ID} = K\% \times RT + (1 - K\%) \times RT_{ID}$$

Where:

Identified peaks:

RT'_{ID}	represents the theoretical peak retention time calculated according to the ‘IntelliUpdate” function, and displayed in the peak identification table of the updated method (after acquisition).

RT	represents the real retention time of the present peak, displayed in the result table, or the interpolated retention time of missing peak according to the reference peak shift (see above equation).
K%	represents the update percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the theoretical retention time of the peak defined in the peak identification table of the acquisition method.

Integration events:

RT'_{ID}	represents the time of the integration events calculated according to IntelliUpdate function, displayed in the integration part of the updated method (after acquisition).
RT	represents the integration event times interpolated according to the reference peak shift (see above equation).
K%	represents the update percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the integration event times defined in the integration part of the acquisition method.

Groups:

RT'_{ID}	represents the calculated group time limits according to column ageing function, displayed in the group identification table of the updated method (after acquisition).
RT	represents the interpolated limit time of groups according to the reference peak shift (see above equation).
K%	represents the ageing percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the theoretical time limits of groups defined in the group identification table of the acquisition method.

The RT time used for the integration events time, group time limits and retention time of the peak defined in the identification table, but missing from the chromatogram is interpolated according to the reference peak shift. Here is the used equation:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_2 - RT_1}{RT_{ID2} - RT_{ID1}}$$

where:

RT	Is the time used in the IntelliUpdate formula.
RT1	Is the retention time of the previous reference peak.

RT2	Is the retention time of the next reference peak.
RTID	Is the theoretical retention time of non-reference peaks (defined in the identification table), or the integration event time, or the time limits of groups.
RTID1	Is the theoretical retention time of the previous reference peak, defined in the identification table?
RTID2	Is the theoretical retention time of the next reference peak, defined in the identification table?

NOTE: If peaks are eluted before the first reference peak, RT1=RTID1= 0 and the index 2 is attributed to the next reference peak.

$$RT = RT2 \times \frac{RT_{ID}}{RT_{ID2}}$$

If a peak is eluted after the last reference peak, RT1 and RT2 represent the retention time of two reference peaks eluted before the peak of interest.

A file is automatically generated after the first acquisition is made with a method using 'IntelliUpdate' function, in which the changes of times (peak RT, group time limits and integration event times) are listed. This file is updated after each acquisition is made with the same method. It is generated in the project directory containing the method, and is named the same as the method it comes from with the METH_CA extension. This file is readable as a text file (Notepad).

Remote Sequence

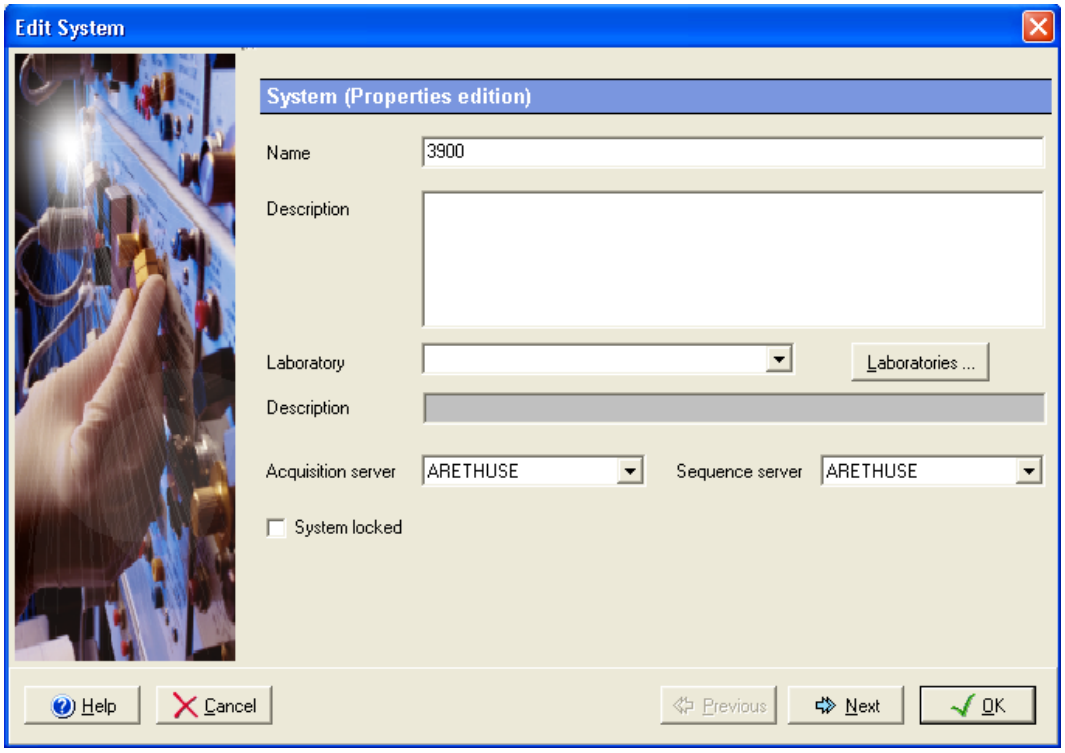
The aim of the 'Remote SequenceRemote Sequence' is to start a sequence on any workstation declared in the domain of work (in the CompassCDS Configuration Manager), and to close the CompassCDS session on this workstation while the sequence is running. It is also possible to disconnect from Windows session without stopping the Remote Sequence.

Configuration

The 'Remote SequenceRemote Sequence' runs as a service of the chromatographic system. One service is created for each system and is named "Remote SequenceRemote Sequence Engine-Systemname" (Systemname represents the name of the system). The services are accessible from the CONTROL PANEL /ADMINISTRATOR TOOLS / SERVICES menu.

At each start of an Remote Sequence, the corresponding service is automatically started on the sequence server, and is automatically stopped at the end of the sequence.

The sequence server is declared in the CompassCDS Configuration Manager in the system object:



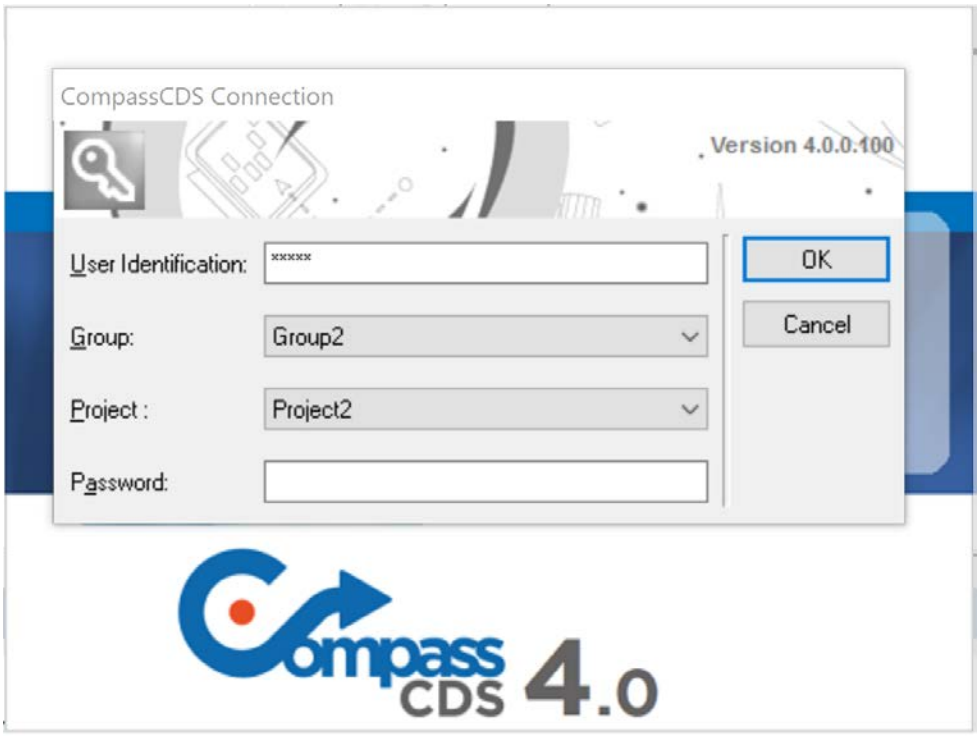
How to Use the Remote Sequence

Connection and Main Screen

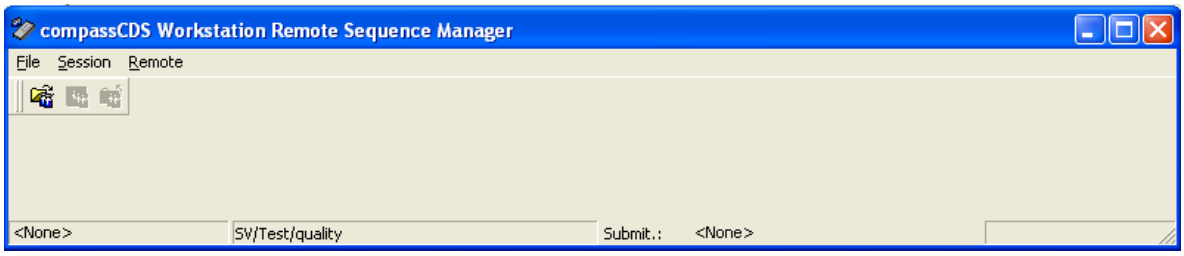
The Remote Sequence software may be opened from CompassCDS Acquisition Menu.

NOTE: The User must have a profile allowing him to start the Remote Sequence Manager (in CompassCDS Configuration Manager: user profile: Sequence / Use remote sequence).

First the logon box is displayed:

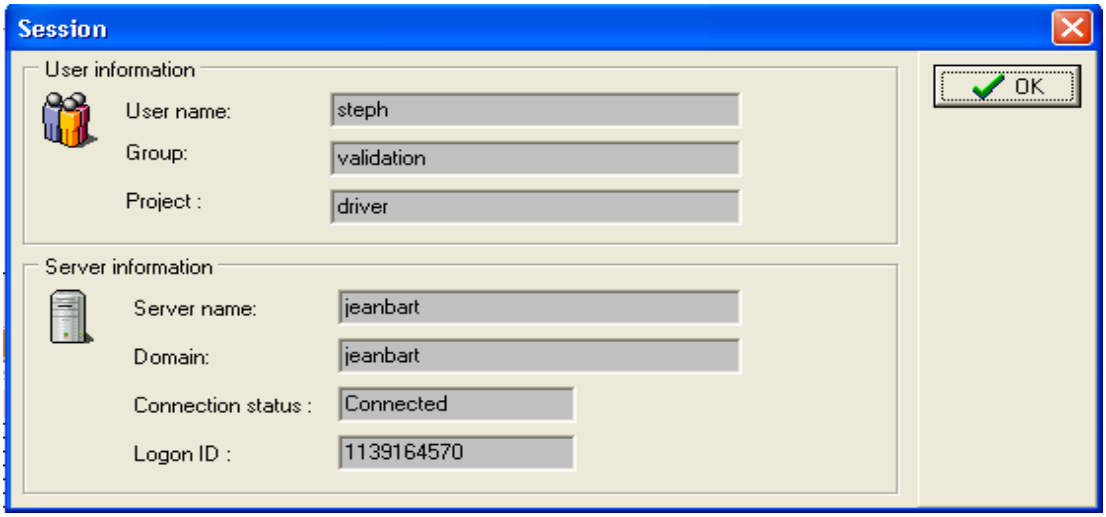


After entering a user name, the user can choose the project/group on which he wants to work and validate. The main screen is displayed:



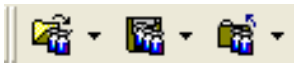
This screen contains three menus:

- **File menu:** allows the user to create, open, save, close a sequence, or quit the Remote Sequence.
- **Session menu:** allows the user to change the Session (New login) or to view properties:



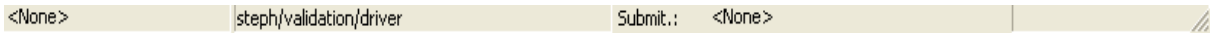
- **Remote menu**: allows access to the Queue status option, which lists all the acquisitions completed and their state. This also allows access to 'System log' option, listing the errors that may have occurred during the acquisition, or mentioning a communication problem with the chromatographic system or other problem.

A Toolbar:



Open sequence, save sequence, close sequence.

A task bar:



Sequence name user/group/project Sequence name by User State

The sequence name content is displayed on a green background, if the sequence displayed has been saved or in red if the changes were not saved.

The second case indicates the logon user/group/project.

The submit case indicates that the current sequence was initiated by 'user'. It has a green background if the current logon is the logon of the user who initiated it, and is red if it was initiated by another user. Note that if several Remote Sequences are opened with the first logon, only the first Remote Sequence opened, has a green background.

The state case shows the sequence state: starting, stopping.

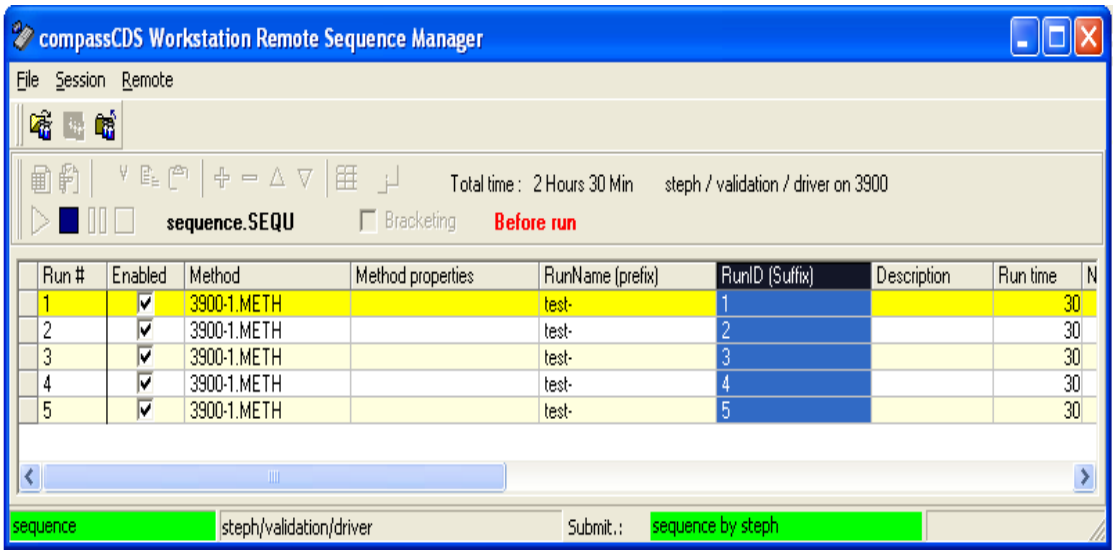
Running a Sequence

The sequence is the same as the sequence in CompassCDS: same grid, same functions. The user should consult the corresponding chapter in the manual (page 145).

External sequence: rules of work

- When a user starts a sequence, he becomes the 'Owner' of this sequence. That gives him all the rights (modify, pause, stop and reset the sequence). Note that changes are only possible when activating the pause button, otherwise the save function is not accessible.

The sequence is displayed as shown in the following picture:


compassCDS Workstation Remote Sequence Manager
File Session Remote
Total time : 2 Hours 30 Min
steph / validation / driver on 3900
sequence.SEQU
Bracketing
Before run
Run # Enabled Method Method properties RunName (prefix) RunID (Suffix) Description Run time N
1 3900-1.METH test- 1 30
2 3900-1.METH test- 2 30
3 3900-1.METH test- 3 30
4 3900-1.METH test- 4 30
5 3900-1.METH test- 5 30
sequence
steph/validation/driver
Submit.:
sequence by steph

The submit field of the task bar is displayed on a green background to remind the user that he started the sequence and that he is its owner.

- If another user connects on another workstation and opens the same sequence, he will only have viewing rights. The submit field of the task bar will have a red background, indicating that this user is not the owner of the sequence and that he has no rights. The stop, pause, reset & start buttons are not accessible to this user. If he makes some changes in the sequence (adds lines for example), these changes will not be taken into account since he is not the owner of the sequence.

Nevertheless 'Non-Owner user' can have rights to change and to save the sequence, if the original owner closes the sequence. However, the non-owner cannot stop the sequence, restart or reset it.

Note that if a non-owner user of a sequence has the 'Stop any running acquisition' profile (declared in the CompassCDS Configuration Manager), he has the full rights (stop, start, save, reset) once the owner has closed the Remote Sequence screen.

Report Printing

The report printing is managed by the workstation on which the Remote Sequence is started. This means that the default printer defined for the Windows user (connected to workstation) will be used for printing, in the sequence. If another user connects to this workstation and the printer associated to his Windows profile is different, reports will be printed on his printer (even if he has not opened the Remote Sequence).

The Windows profile of the user connected to the workstation defines the printer.

To print reports, the workstation must always be connected under a Windows session. If no user is connected on a Windows session, acquisitions will be performed, but no printing will be done.

NOTE: To change Windows log-on, select the "Close all programs and log on as a different user." This is the option in the start menu to avoid stopping the computer.

Retention Index

CompassCDS has an option enabling retention indices calculation. Retention index is defined by reference to two standards of homologous series, whose peaks bracket the compound of interest. Calculation is based on Kovats principle (for alkanes with isothermal temperature) extended to other chemical series (alkenes, esters…) and temperature programs.

Reference compounds can be either analyzed simultaneously to unknown compounds, or separately, provided, that analytical conditions remain identical.

This option allows identification not only with retention time, but also with retention indices.

Configuration

To activate this option, the user must be assigned a CompassCDS Configuration Manager user profile. Check the "Edit peak identification parameters" and "Retention index" options in the "Method" subdirectory of the user profile.

Two options are then available in the "Peak identification" part of the method: "Retention index" and "Identification using index".

Check the "Retention index" box to use the retention index option.

- A column appears in the identification table: Ret. Index. It allows the user to enter retention indices in the peak identification table.
- A new menu RETENTION INDEX appears in the main toolbar.
- The option "Identification using indices" becomes active. If it is checked, two additional columns appear in the identification table: Abs window (ret.ind), Window % (ret.ind). Abs window (min) and Window % columns disappear.

Reference Table Building

To calculate retention indices in an unknown chromatogram, a "Reference table" must be created. In a homologous series of chemical compounds, this table links retention time to retention index.

A reference table consists of two parts:

- Analytical conditions of chromatogram acquisition.
- Reference identification table, which lists the entire homologous series information (retention time, retention index, identification window, etc.).

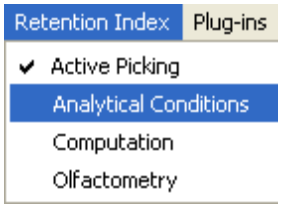
Reference Analytical Conditions

Retention index calculation can only be done between chromatograms whose analytical conditions are identical. So, reference analytical conditions must be created.

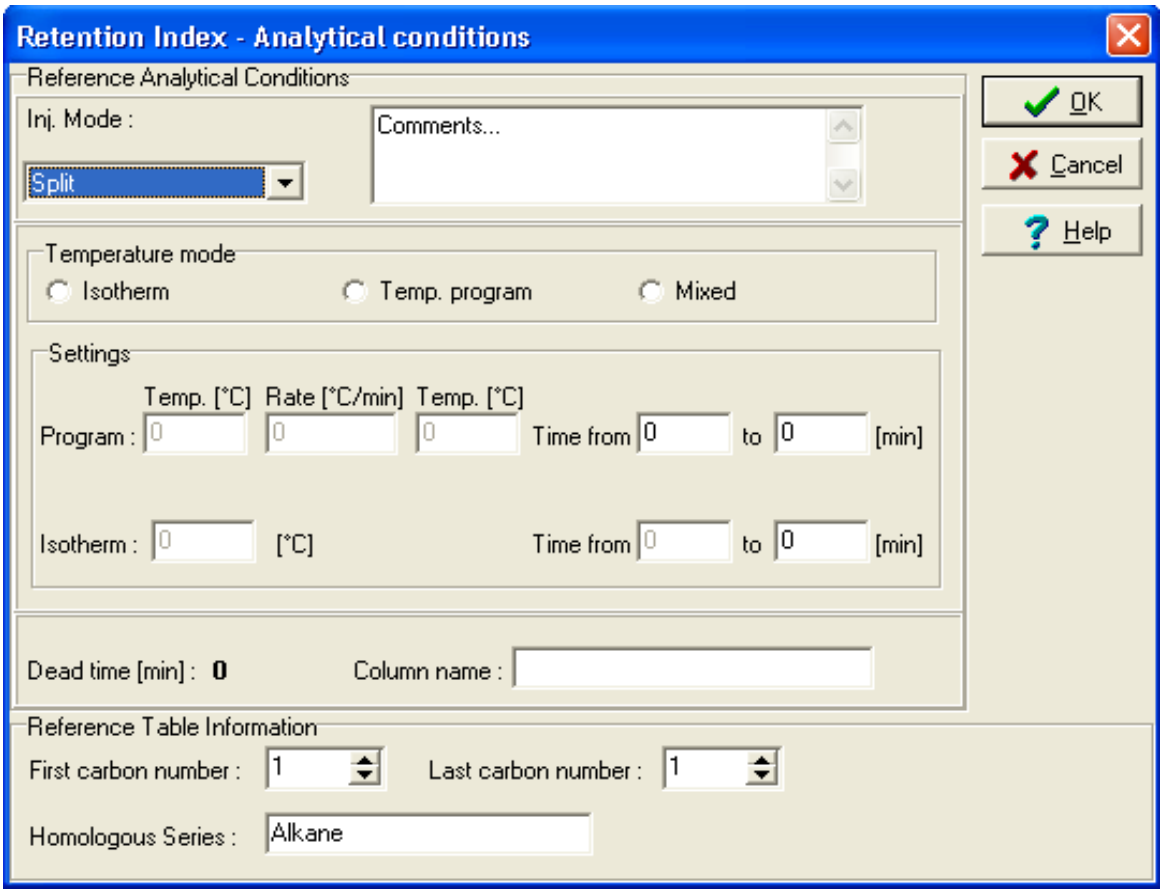
Open a method.

In the peak identification table, check "Retention index" option and possibly the "Identification using index" one.

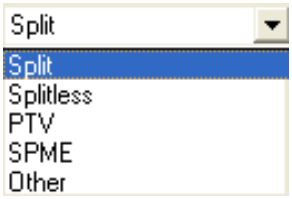
Select the RETENTION INDEX / ANALYTICAL CONDITIONS menu.



The following screen appears:



Inj mode: select the injection mode among: Split, Splitless, PTV, SPME or Others



Comments: Enter comments if necessary

Temperature mode: select temperature conditions of the acquisition. Three temperature modes are available:

- **Isotherm:** enter the temperature.
- **Temp. Program:** enter initial and final temperatures and the rate. Only one rate is allowed.
- **Mixed:** a rate can only be followed by an isothermal level. Enter temperature, rate, and initial and final program time.

Dead time: The column dead time is imported from the acquisition part of the method, it is impossible to enter this data manually.

Column name: enter column name.

Reference table information: to specify reference compounds.

- **First carbon:** carbon number of the first reference compound.
- **Last carbon:** carbon number of the last reference compound.
- **Homologous series:** name of homologous series.

NOTES: If the last carbon number is less than the first, it appears on a red background to inform user of the inconsistency.

Each compound within the defined range (from first carbon number to last carbon number) must be present, in order to construct the Reference Identification Table

Save the method when all fields have been filled out.

Reference Identification Table

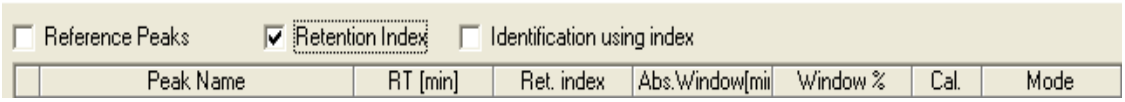
When reference analytical conditions have been defined in the method, reference chromatogram (chromatogram containing the peaks of interest of the homologous series) can be either reprocessed (F6) or acquired with this method.

Then reference peak identification table can be built.

Peaks can be identified according to their retention time or their retention index:

If the Retention index option is checked and identification using index is unchecked, peaks are identified according to their retention time.

The following identification table appears:



Peak name: compound name.

RT: theoretical retention time of the compound.

Ret. Index: theoretical retention index of the compound.

Abs window (min): absolute identification window in minutes (according to retention time).

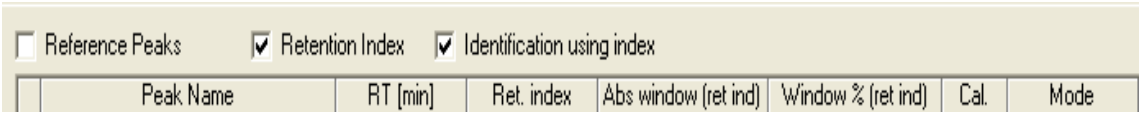
Window %: relative identification window in % (according to retention time).

Cal: check this box if the compound must be used for calibration.

Mode: identification mode.

If the Retention index AND Identification using index options are checked, peaks are identified according to their retention index.

The following identification table appears:



Peak name: compound name.

RT: theoretical retention time of the compound.

Ret. Index: theoretical retention index of the compound.

Abs window (ret ind): absolute identification window for retention indices.

Window % (ret ind): relative identification window in %, for retention indices.

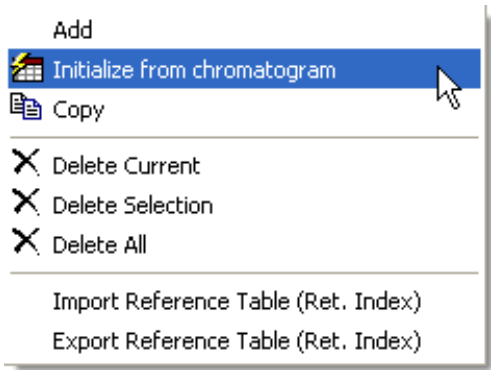
Cal: check this box if the compound must be used for calibration.

Mode: identification mode.

Once identification mode has been selected, identification table can be filled-in either with popup menu or peak picking:

- With identification table popup menu:

Initialize from chromatogram option fills in the identification table with chromatogram information.

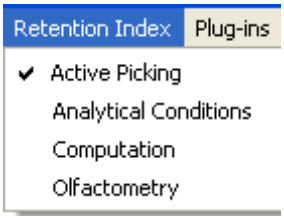


Peaks are automatically named and the retention index and filled according to what has been specified in the reference table information (name, first and last carbon).

Once peaks have been identified, the user must complete the other fields of the identification table.

- With peak picking from the chromatogram.

Active Picking option is accessible in the RETENTION INDEX / ACTIVE PICKING menu. It allows peak selection directly on the chromatogram.



Selected peaks are automatically named with homologous series names, and retention indices filled according to limits defined in the reference table information.

Peaks must be chronologically selected but if an error occurs, a chronological sorting is proposed.

Once peaks have been identified, the user must complete the other fields of the identification table.

NOTES: If data about peaks (name, retention time, retention index…) are known when the method is built, the identification table can be manually completed.

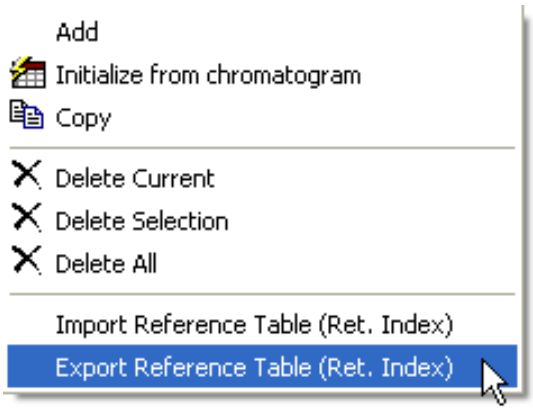
If a chromatogram is processed in retention index mode, and that it is subsequently reprocessed by a user who does not own the retention index profile, a sentence informs the inconsistency in the identification table.

Reference Table Export and Import

- Export:

Once reference analytical conditions and identification table have been built in a method, the reference table can be created in order to be used in other methods.

To export the reference table, select the popup menu Export reference table in the peak identification table of the reference chromatogram or method.

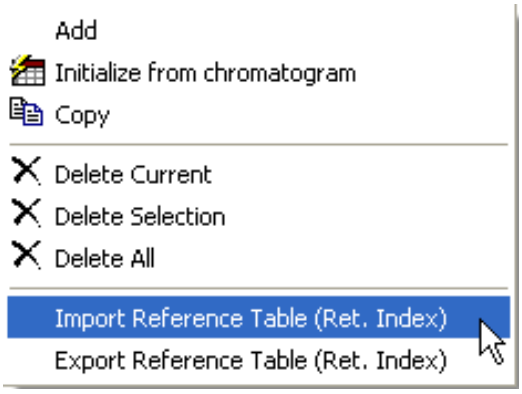


A file named ‘Chromatogram name.csv’ and readable in Excel is created, in the directory defined by the user during the export step. It contains the reference analytical conditions and the identification table.

- Import:

The reference table can be imported either in a method or in a chromatogram in order to process unknown chromatograms with retention indices.

To import the reference table, select the popup menu Import reference table of the peak identification table.



Retention Index Calculation

In the peak identification table, check "Retention index" box and if necessary "Identification using index" option.

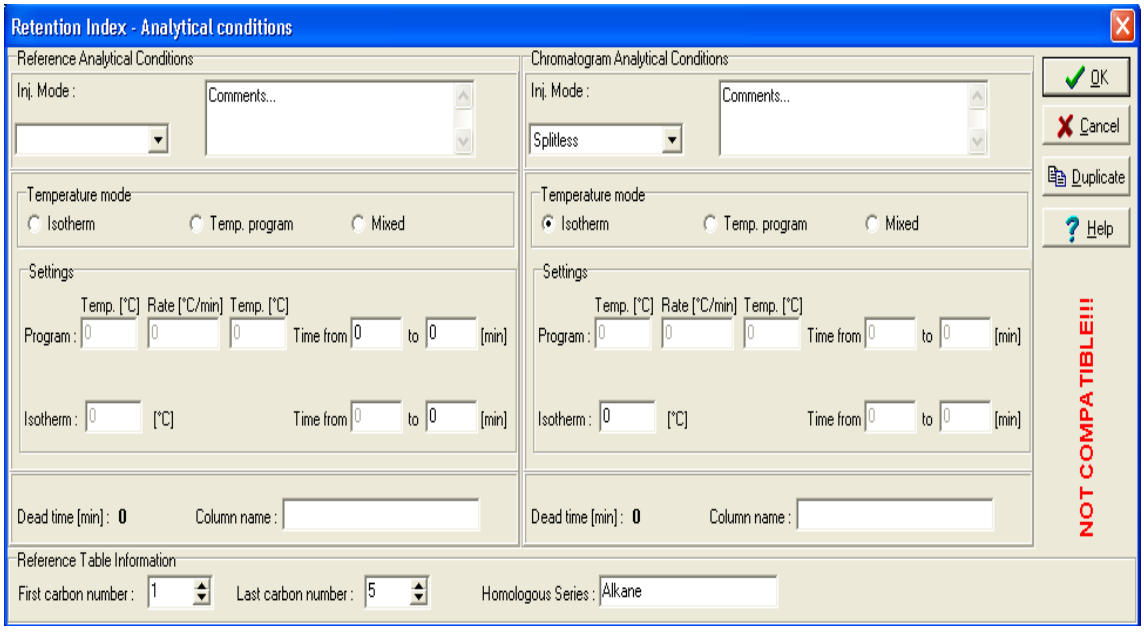
Processing Method

To calculate retention indices in a chromatogram, analytical conditions must remain identical.

Unknown chromatograms method must contain retention index reference parameters (table + analytical conditions). So, it is mandatory to either import a reference table via the popup menu "Import reference table" in the identification table, or to reprocess the chromatogram with a method which contains a reference table.

The identification table is then filled in with reference chromatogram peaks.

Select RETENTION INDEX / ANALYTICAL CONDITIONS menu, the following screen appears:



Reference analytical conditions: It contains the analytical conditions of the reference. This part cannot be modified in the chromatogram.

Chromatogram analytical conditions: It contains the analytical conditions of the unknown chromatogram.

Reference table information: It contains all information about homologous series of chemical compounds.

Index retention calculation is processed only if analytical conditions between reference and chromatogram are identical. A message COMPATIBLE or NOT COMPATIBLE!!! is displayed in order to advise the user if calculation can be done or not.

NOTE: If a chromatogram is acquired with a method containing retention index parameters (reference table, analytical conditions), the Chromatogram Analytical Conditions part is identical to the Reference Analytical Conditions. If reprocessing a chromatogram not acquired with retention index parameters with a method containing Retention Index parameters, the user has to complete the Chromatogram Analytical Conditions screen.

The

button copies reference analytical conditions into chromatogram ones.

As soon as COMPATIBLE is displayed, the user can process his chromatogram (or).

Calculation

The retention index calculation depends on analysis temperature program (Isotherm, Program, and Mixed)

- Isotherm: $$i_x = 100 * \frac{\log(t'_x) - \log(t'_n)}{\log(t'_{n+1}) - \log(t'_n)} + 100 * n$$
- Temp. Program: $$i_x = 100 * \frac{t_x - t_n}{t_{n+1} - t_n} + 100 * n$$

Where:

ix: retention index of the peak of interest,

t'_x: relative retention time of the peak of interest,

t'_n: relative retention time of the previous reference peak,

t'_{n+1}: relative retention time of the next reference peak,

t_x: retention time of the peak of interest in minutes,

t_n: retention time of the previous reference peak in minutes,

t_{n+1}: retention time of the next reference peak.

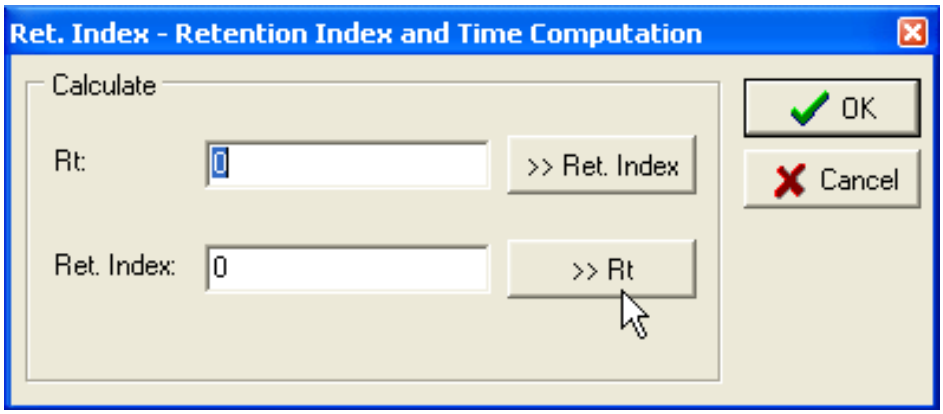
Where relative retention time (t') = retention time (t) - Dead time

- Mixed: In this program, a rate can only be followed by an isothermal level. During the rate, calculation is done with the temp. program formula. During the isothermal level, calculation is done with isotherm formula. If the peak of interest is bracketed with reference compounds

whose retention times are on different temperature programs, calculation is done with temp. program formula.

According to peak identification table information, the CompassCDS Chromatography Data System proposes an option which allows calculation of retention index from retention time, and the reverse calculation.

Select the RETENTION INDEX / COMPUTATION menu, the following screen appears:



If retention time is entered, select the

button, retention index will be calculated.

If retention index is entered, select the

button, retention time will be calculated.

NOTE: Calculations are allowed only in the retention time range or in the retention indices range defined in the identification table.

Variables

Two global variables are available:

Analysis Type [ANALYSISTYPE]: the type of analysis chromatogram or olfactogram.

Reference table name [REFTABLENAME]: the reference table name imported in the peak identification table.

Three peak variables are available to display calculation results.

RT Ind. [RETENTION_INDEX]: retention index of the compound.

Ret. Ind. offset [RETIND_OFFSET]: offset between theoretical and experimental retention indices.

Corr.Ret.Ind [RETIND_CORRECT]: corrected retention index according to reference compounds.

Results

Results are displayed in the Results-Peak report part of the chromatogram.

Select the "Report properties" popup menu to display Ret Ind., Ret Ind. Offset, Ret Ind. correct variables.

NOTE: If calculations have been processed within incompatible analytical conditions, the retention index column will appear in red.

On the chromatogram, compounds of the homologous series identified are named automatically.

CompassCDS Report Editor Report Style

Identification parameters are contained in the 'Method' object of the CompassCDS Report Editor Report style.

Results are contained in the 'Peak result' part of the CompassCDS Report Editor Report style.

CompassCDS ASCII Import

The CompassCDS ASCII Import allows converting ASCII data (.txt or .csv) into CompassCDS data files. This option is installed by default with CompassCDS; it is accessible via the FILE / IMPORT / ASCII FILES menu or the icon.

The details of this application are described in a separate user's guide, available in the CompassCDS / Manuals directory.

CompassCDS Print manager (PDF Export)

The CompassCDS Print Manager allows the user, when it is used as a post-processing, to combine printings and exports as PDF of the same chromatogram. Different printers, report styles and output paths can be chosen in the same configuration table. It also allows to export chromatograms as PDF and to choose the path where they are going to be stored on the computer.

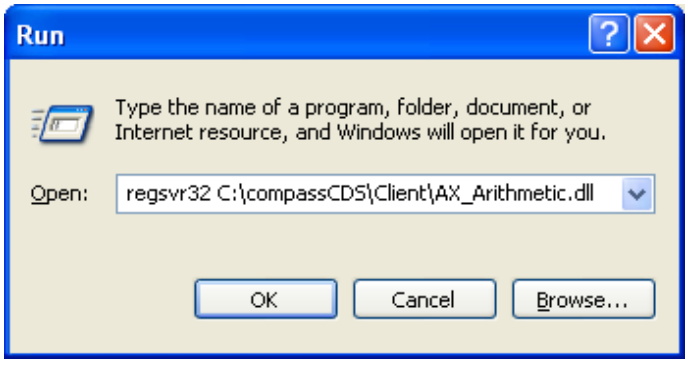
The details of this application are described in a separate user's guide, available in the CompassCDS / Manuals directory.

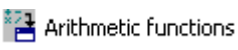
CompassCDS Arithmetic functions

The Arithmetic functions allow the user to realize operations (Addition, Multiplication, Subtraction, Division, and Weighted sum) between either chromatograms or chromatogram and real numbers.

The Arithmetic functions option is not installed by default with CompassCDS. The program is nevertheless available in the CompassCDS /Client directory.

To install it, select the START / RUN menu, enter 'regsvr32 ' then drag and drop the AX_Arithmetic.dll file from the COMPASSCDS / CLIENT directory:



To access the Arithmetic functions options, select the icon then the  sub-menu. The details of this application are described in the CompassCDS Arithmetic Functions Plug-in User Guide..

Procedures

This section gives actual examples of various procedures:

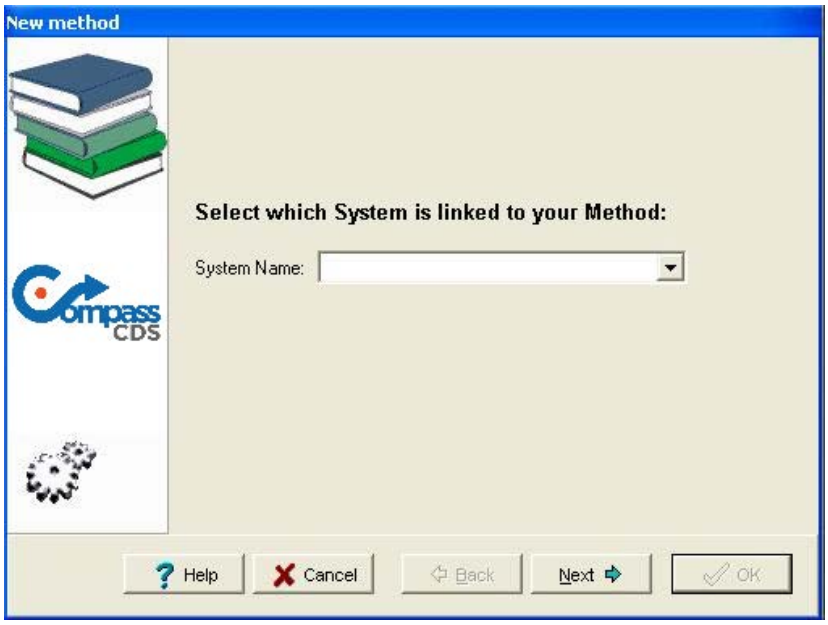
- How to acquire a chromatogram.
- How to program sequential analyses: the sequence.
- Creating a process method (integration, identification, quantification and printing).
- How to reprocess a chromatogram (integrate, quantify, print a report for a standard or an unknown sample).
- How to create a calibration curve.
- How to create a customized report.

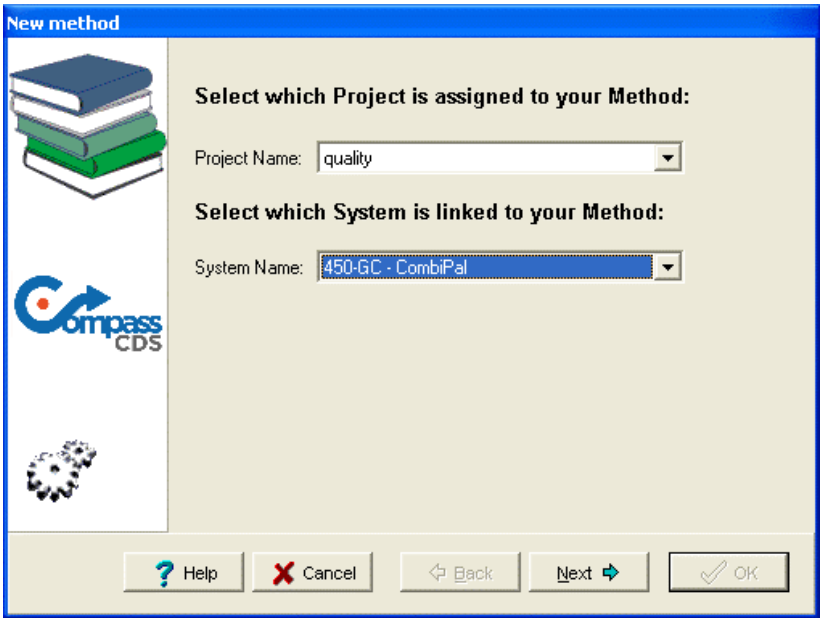
How to Acquire a Chromatogram

1. First create a method containing at least the control and acquisition parameters. Once the method has been created and saved, the acquisition can be started.

   Select FILE / NEW / NEW METHOD

   One of the following screens is displayed, depending on the way you log on to the CompassCDS Chromatography Data System, either in “all projects” or in a defined project.





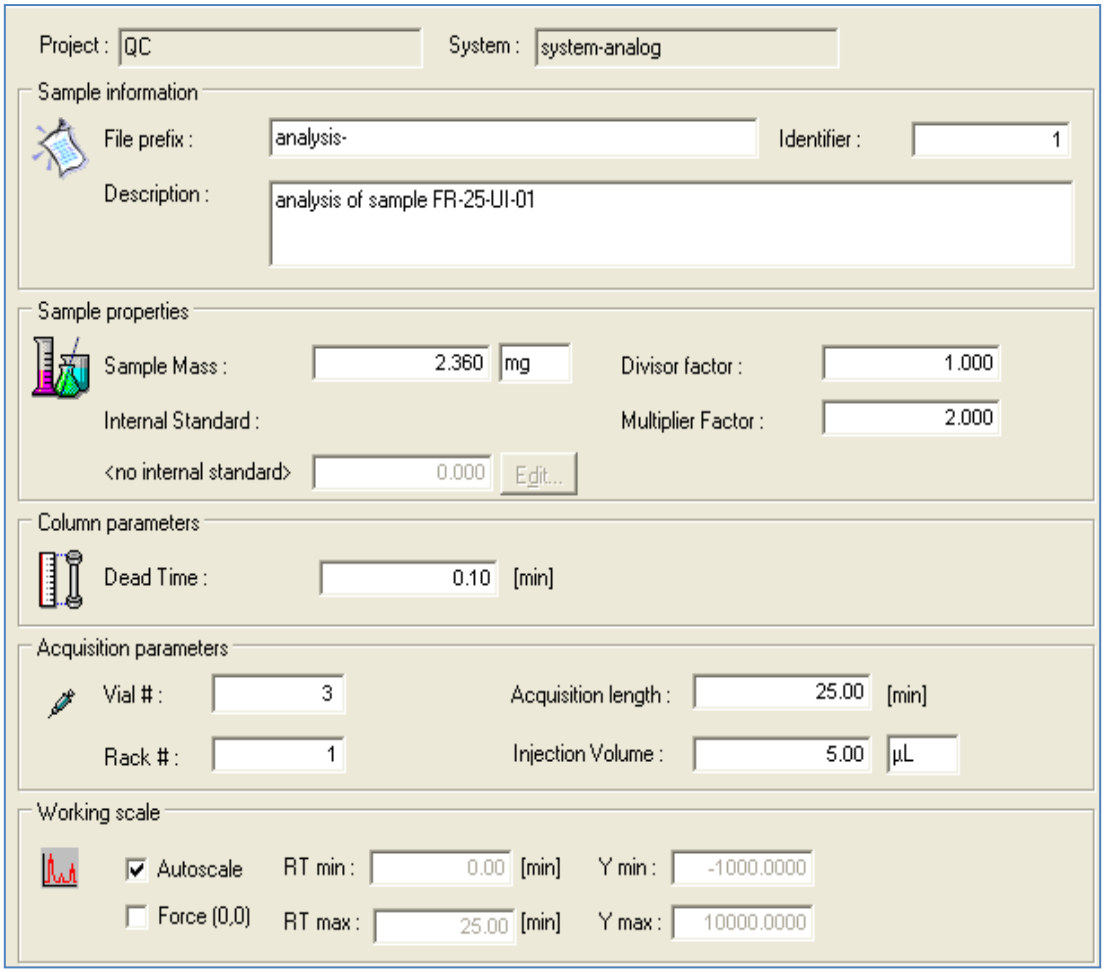
- Define either the name of the project linked with the method and the name of the system, or only the name of the system. The method is created and then displayed in the browser.
- Enter the control and acquisition parts of the method:

Control: This section depends on the chromatographic system and whether it is controlled or not by CompassCDS. Define:

The acquisition rate (number of points acquired per second).

- Start mode: “start on trigger” if the start signal is triggered by user (click on the chromatograph’s start button) or by an autosampler, or “start immediately” if CompassCDS triggers the start.
- The control parameters in the case of a controlled system.

  Acquisition:

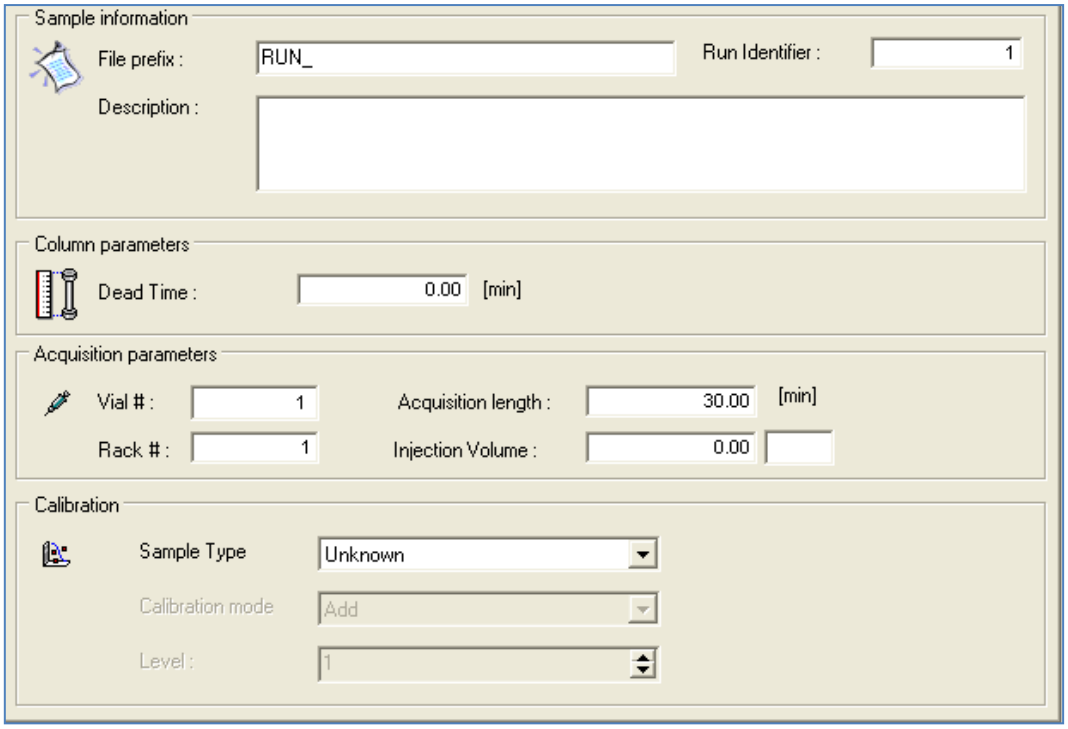


Complete at least the following fields: File prefix and Identifier, corresponding to the entire chromatogram name, and Acquisition length.

Save the method.

Start the acquisition (see page 139)

Press the button. The following screen is displayed:



If the system is using an autosampler controlled by the CompassCDS, define the injection volume, the vial position, the rack number (if required, otherwise leave at 0 as default), then click on the START button. If an Internal START is defined, CompassCDS controls the START; if an "external START" is defined (manual injection), inject and then press the START button on the chromatograph.

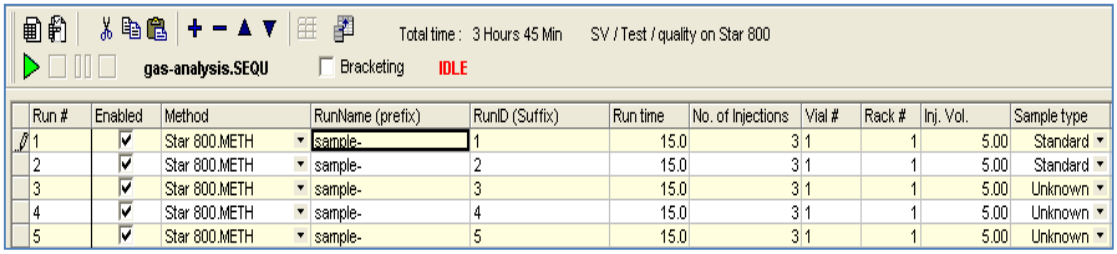
How to view the current acquisition:

In the "system" tab, select the system (click with the mouse on the left of the system name).

How to Define a Sequence for Analysis Execution

1. Define an analysis method. A minimal method is enough for an acquisition (page 241), but it is also possible to process automatically (identification, quantification, report printing, etc.) by using a more elaborate method.

   Create a sequence: menu FILE / NEW / NEW SEQUENCE, complete the displayed creation wizards (page 145), by entering the used system name, the number of lines (corresponding to the number of samples) and the sequence name. The sequence is displayed.
   Complete the sequence (page 147).



Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type
1	☑	Star 800.METH	sample-	1	15.0	3	1	1	5.00	Standard
2	☑	Star 800.METH	sample-	2	15.0	3	1	1	5.00	Standard
3	☑	Star 800.METH	sample-	3	15.0	3	1	1	5.00	Unknown
4	☑	Star 800.METH	sample-	4	15.0	3	1	1	5.00	Unknown
5	☑	Star 800.METH	sample-	5	15.0	3	1	1	5.00	Unknown

Some fields must be completed before starting the sequence:

The method name,

The RUN NAME,

The RUN ID,

The RUN TIME.

All this information is automatically imported from the method acquisition part if defined.

Specify in the ‘sample type’ column whether the chromatogram is a ‘blank to be subtracted’, a ‘standard’ (for automatic creation of calibration curve, choose this option only if the calibration mode defined in the method is curve) or an ‘unknown’. For standard chromatograms, it is compulsory to complete the ‘level’ and the ‘calibration’ fields.

Start the sequence by clicking the button.
To view the current acquisition, select the “system” tab and then the system name.
After each acquisition, a chromatogram is generated and available for processing (FILE / OPEN / OPEN CHROMATOGRAM). If standards have been defined the calibration curve is generated, display it in the ‘calibration’ tab, by using the FILE / OPEN / OPEN CALIBRATION CURVE menu.

How to Build a Process Method

(Integration, identification, quantification and printing)

It is recommended that the process sections of the method to be done after the acquisition of a chromatogram, typical of the analysis to be performed. In the first step, the parameters are in the chromatogram method; once completed the method is extracted from the chromatogram and a method file is generated. This method will be used to acquire and to reprocess other chromatograms.

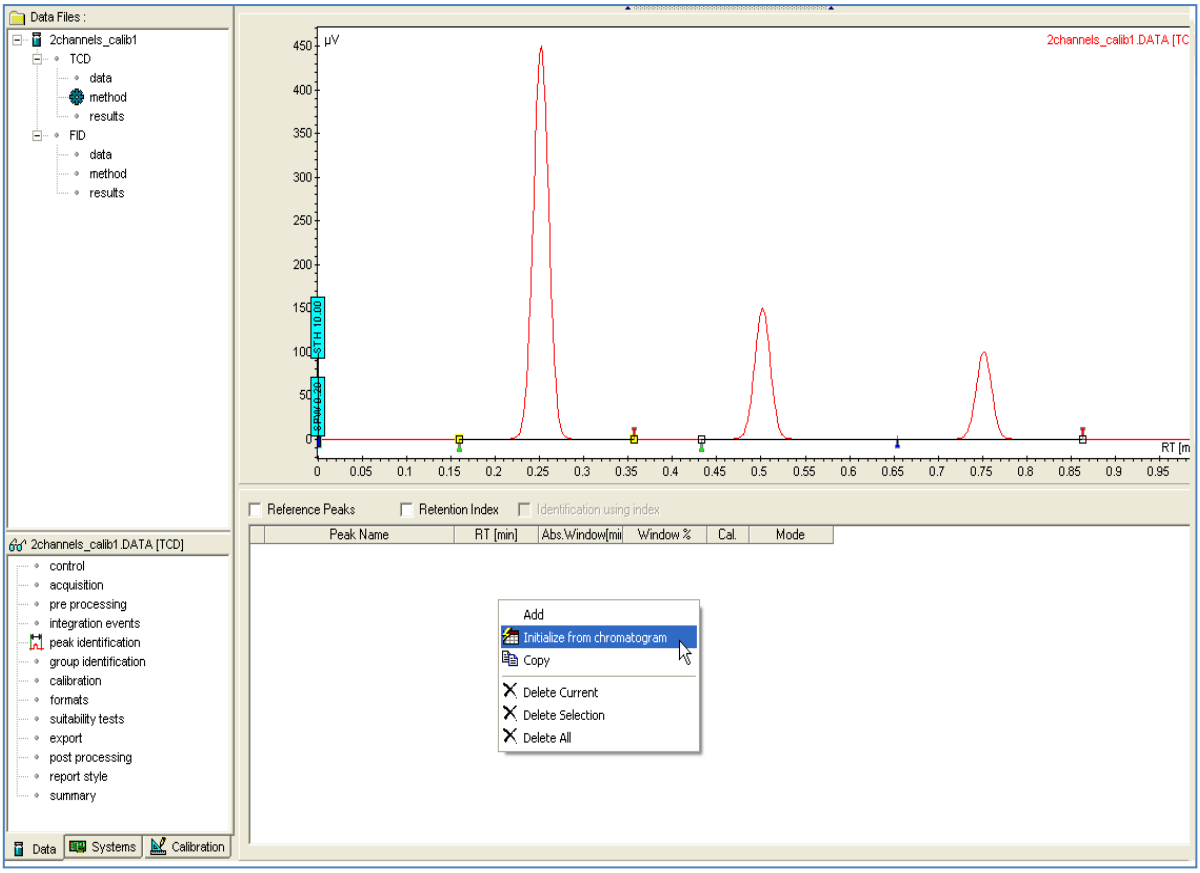
Remember that a method file contains all of the useful information, from acquisition to report printing via integration, identification, quantification etc.

1. Acquire a chromatogram with a minimal method (refer to page 241).

   Open the generated chromatogram, select the method part.
   Complete the following parts:

   - Integration: define the integration events to obtain the optimum integration (See page 43 for the details of each event). Once an event is defined, click on the icon to apply changes. Changes are immediately taken into account and integration results are available for viewing in the chromatogram results part.
   - Peak identification:

   Click on the right mouse button and select the ‘Initialize from chromatogram’ option.



The retention times of all integrated peaks of the chromatogram are displayed. Type a name for the peaks of interest and delete any lines which are not of interest (select the entire line, click on the right mouse button, Delete Current). Define the identification windows and the identification mode (refer to page 65).

- Group identification: refer to page 73.
- Calibration: The user must configure the calibration parameters in this subsection.

Two examples are described:

Example 1: Response in area, external standard, with a calibration curve of 3 levels with averaging, results displayed in µg/L, process unknown peaks with a response factor of 0.59.

- Click on “external standard”,
- Click on the Initialize from peak ID button, to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatic.
- Define the parameters: area response, curve response factor, standard quantities in the identification table (define the column number using the parameter “level number”, check the “average levels” box to, average points of the same level before drawing the curve), enter a curve name (the generated file will contain all the calibration curves generated, by compound), define the unknown peaks process.

The calibration method section is now complete. To use this method, to acquire or reprocess other chromatograms, it must be extracted. For this save it via the menu: FILE / SAVE AS / SAVE METHOD AS. Give a name to the method. The method is created for the system associated with the chromatogram used for its creation.

Example 2: Response in height, internal standard with normalization to 75.8%, subtracting the internal standard(s) quantity (ies) of final results, use response factors entered by user, reprocess the unknown compounds as one of the identified and quantified compound.

Click on “internal standard”

Click on Initialize from peak ID button to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatic.

The user must define which peak(s) is (are) internal standard(s), by checking the corresponding box in the calibration table.

Set the other parameters: responses in height, manual factors, check the “normalize to” box and enter the normalization percentage, check the ‘subtract ISTD mass’ to subtract the internal standard quantity (ies) from results. In the unknown compounds process, select “reference component” and define in the “Standard” box the name of the associated internal standard.

- The calibration method section is complete. To use this method, to acquire or reprocess other chromatograms, it must be extracted. For this save it via the menu: FILE / SAVE AS / SAVE METHOD AS. Give a name to the method. The method is created for the system associated with the chromatogram used for its creation; the control section must still be completed.

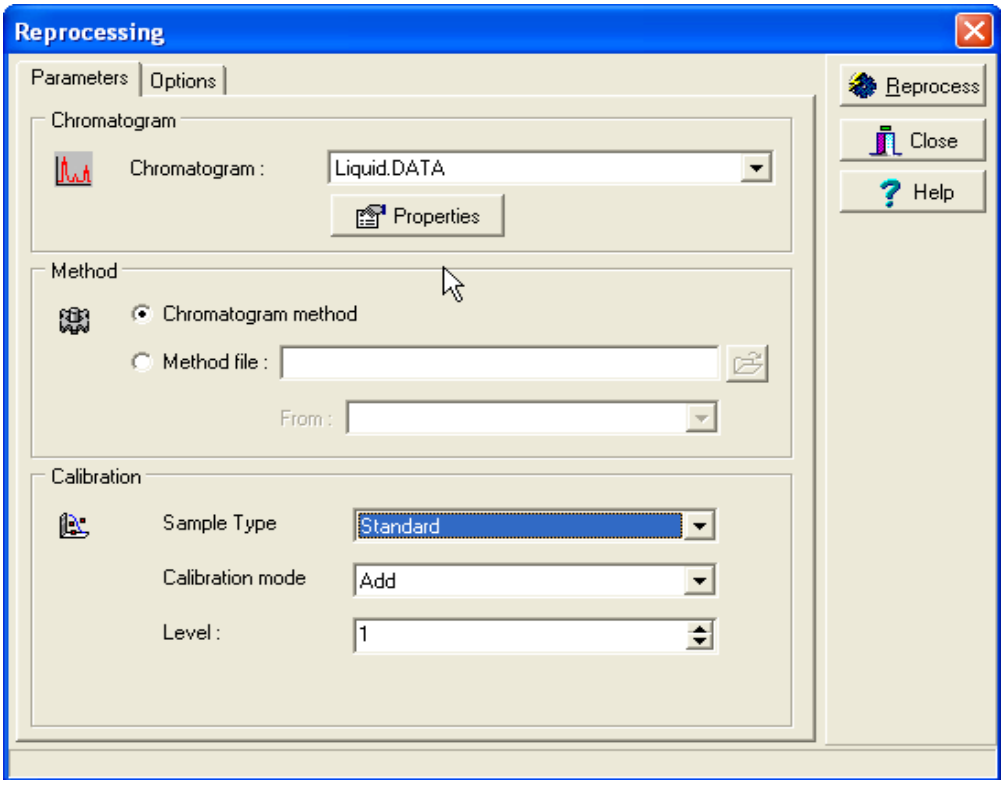
How to Reprocess a Chromatogram

(To integrate, quantify, print a report for a standard or an unknown sample)

There are two ways to reprocess a chromatogram, the reprocessing of an individual chromatogram, or the reprocessing of a series of chromatograms using a reprocessing list.

Individual chromatograms reprocess:

1. Open the chromatogram to reprocess.
2. Menu PROCESSING / REPROCESS, complete the following screen (reference to ‘Single Reprocessing’ section).

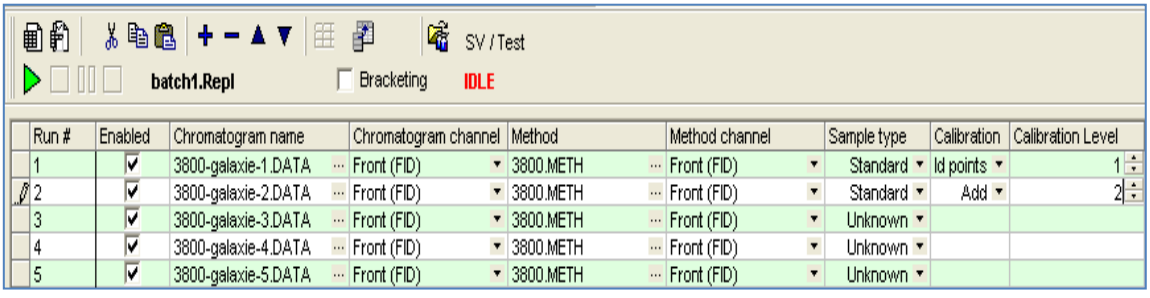


In the method section, choose the chromatogram method or another method selected in the field “method file”. In the calibration part, specify the sample type: an unknown or a standard of level (I). If the chromatogram is a standard (calibration point generation), the user can choose to overwrite an existing curve by checking the “Clear old points” box, to overwrite all the points of the same level already built by checking the “Clear this level only” box or to add the point to an existing curve (do not check anything). If the chromatogram is an unknown, do not check anything.

3. Click on the reprocess button. When the ‘Processing done’ message is displayed, the chromatogram is reprocessed.
4. Click on the Close button. The results are immediately updated in the chromatogram.

Reprocess simultaneously several chromatograms (refer to the Reprocessing Several Acquisitions: The Reprocessing List section, page 176).

Create a reprocessing list. Menu FILE / NEW / NEW REPROCESSING LIST.


SV / Test
batch1.Repl
Bracketing
IDLE
Run # | Enabled | Chromatogram name | Chromatogram channel | Method | Method channel | Sample type | Calibration | Calibration Level
1 | 3800-galaxie-1.DATA | Front (FID) | 3800.METH | Front (FID) | Standard | Id points | 1
2 | 3800-galaxie-2.DATA | Front (FID) | 3800.METH | Front (FID) | Standard | Add | 2
3 | 3800-galaxie-3.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown
4 | 3800-galaxie-4.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown
5 | 3800-galaxie-5.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown

Select in the ‘Chromatogram name’ field, the chromatograms to be reprocessed, specify the method name to be used in the corresponding field, complete the ‘sample type’ field (specifying whether the chromatogram is an unknown or a standard). If the chromatogram is a standard, the ‘Calibration level’ and ‘Calibration’ columns must be completed.

Depending on the parameters defined in the method, fill in the other fields as necessary.

Start the reprocessing list by clicking on .
Once the reprocess is completed, open the chromatograms and view the results or checkthe printed report if any printing was defined in the method.

NOTE: Chromatograms selected in a reprocessing list must be closed in CompassCDS to be reprocessed

How to Build a Calibration Curve

A calibration curve can be created either automatically during the acquisition, or after by reprocessing chromatograms.

Creating a calibration curve during the acquisition: (see page 160)

Create a method; fill in at least the identification and calibration parts, as mentioned in “The different Parts of the Method” section.

Acquire chromatograms, either using a Quick Start or a sequence (see page 139).

In the case of a simple acquisition, complete the ‘Quick Start’ windows in the ‘calibration’ field; define the sample type using the scrolling menu (standard of level 1, standard of level 2, etc.). Check ‘clear old points’ to overwrite an existing calibration curve, ‘clear this level only’ to overwrite all the points of the same level or do not check anything to add the point to the existing calibration curve. Start the acquisition and the corresponding calibration point is created.

In the case of a sequence, specify in the ‘Sample Type’ column which chromatograms are standards by selecting ‘standard’. For all these standards, it is compulsory to associate a corresponding level number in the column ‘Level’ and select the appropriate option in the ‘calibration’ column: ‘clear old points’ to overwrite an existing calibration curve, ‘clear this level only’ to overwrite all the points of the same level or do not check anything to add the point to the existing calibration curve.

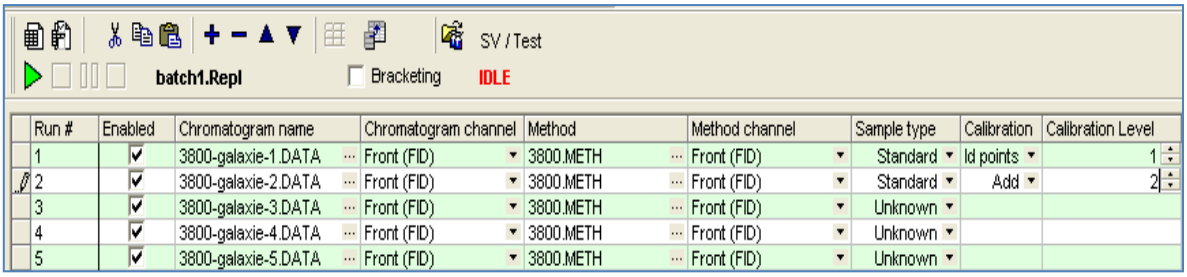
Creating a calibration curve after the chromatogram acquisition (see page 160)

Create a method; fill in at least the identification and calibration parts, as mentioned in ‘The different Parts of the Method’ section.

The process can be made in two ways: using the REPROCESS function to reprocess one chromatogram after the other, or using a Reprocessing list to reprocess several chromatograms.

REPROCESS: The chromatograms to reprocess must be open, select the menu PROCESSING / REPROCESS and follow the instructions defined in the Single Reprocessing section.

Reprocessing list (see page 176)



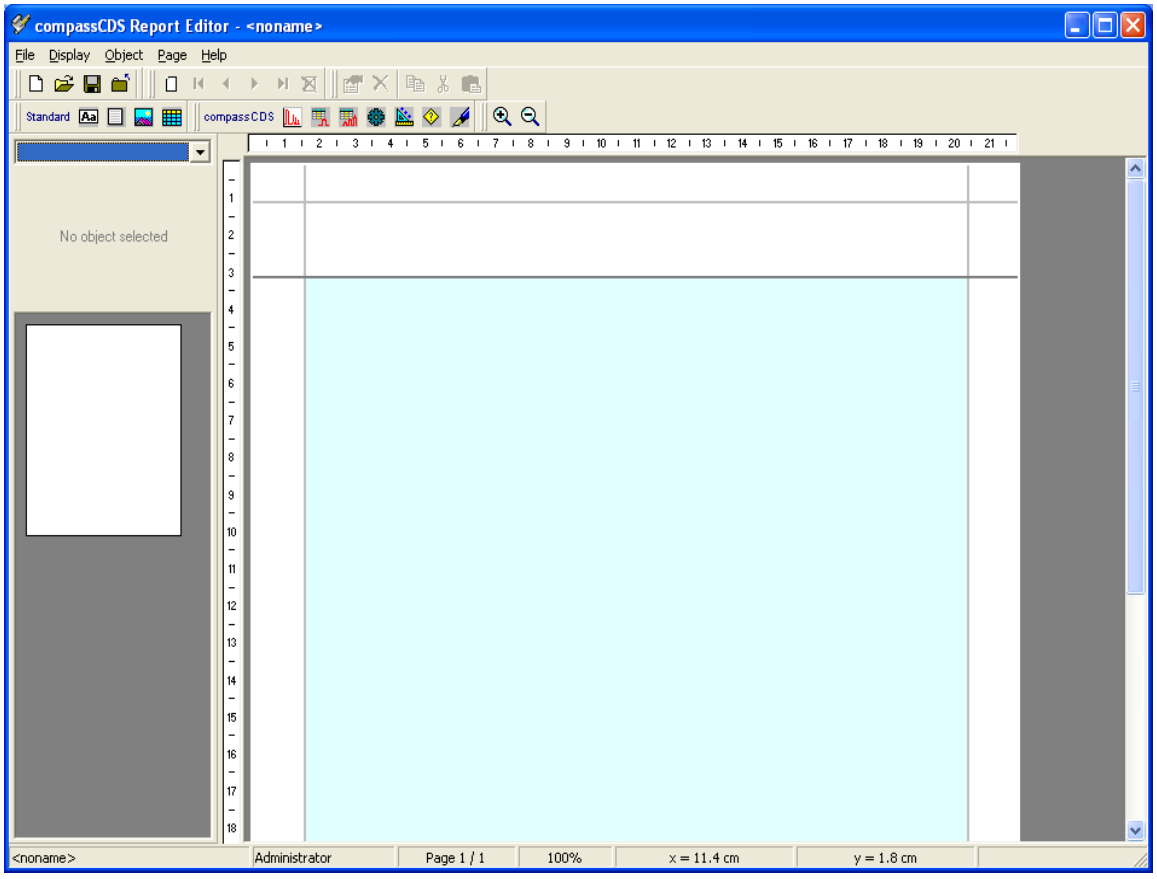
Run #	Enabled	Chromatogram name	Chromatogram channel	Method	Method channel	Sample type	Calibration	Calibration Level
1	☑	3800-galaxie-1.DATA	Front (FID)	3800.METH	Front (FID)	Standard	Id points	1
2	☑	3800-galaxie-2.DATA	Front (FID)	3800.METH	Front (FID)	Standard	Add	2
3	☑	3800-galaxie-3.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		
4	☑	3800-galaxie-4.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		
5	☑	3800-galaxie-5.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		

Select the chromatograms to be reprocessed in the ‘Chromatogram name’ column, specify the name of the method to be used in the corresponding field and complete the ‘sample type’ column. For the standard chromatograms do not forget to fill in both ‘Calibration level’ and ‘Calibration’ columns.

Depending on the parameters defined in the method, fill in the other fields.

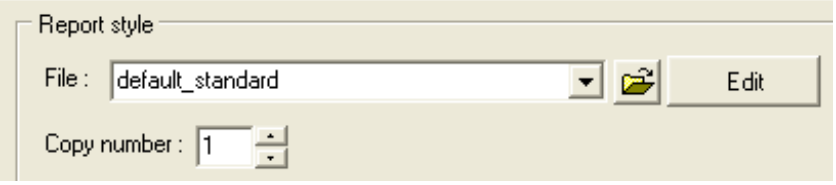
How to Print a Customized Report

1. A report template must first be created, define the objects to be printed: chromatogram, result table, calibration curve, text, etc. This template is created from CompassCDS Report Editor. Select the FILE / NEW / NEW REPORT STYLE menu. The CompassCDS Report Editor interface is displayed:



Define the template (refer to the CompassCDS Report Editor user’s Guide), save it and close the CompassCDS Report Editor.

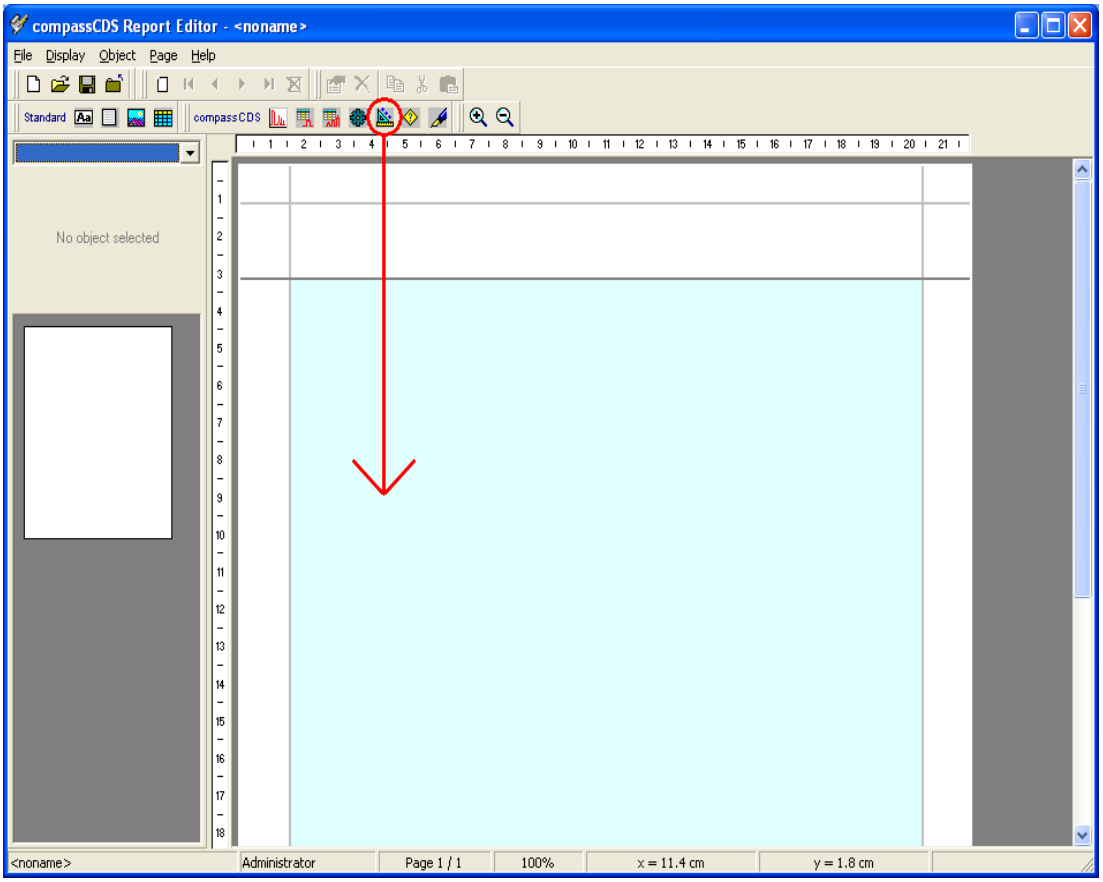
In the CompassCDS Chromatography Data System, in the ‘Report style’ part of the method, select the template name in the ‘File’ box, and define the number of reports to be printed.



Report printing is automatic during an acquisition (QUICK START), a sequence, a reprocessing list or a reprocess using the function, using a method in which a template and at least one printing is specified. Nevertheless, it is possible to do all these functions without printing the report by un-checking the printing option in the “Options” tab of the REPROCESS or of the QUICK START or in the “Method properties” column of the sequence or of the reprocessing list.

How to Print a Calibration Curve

1. Create a calibration curve (see “The Calibration Curves section” page 160).
2. Create a report style in the CompassCDS Report Editor, for which the calibration curve object is specified.



Open a chromatogram whose method contains a calibration curve name (‘Calibration’ section) and then print by clicking on the icon.

Two options are available:

- Printing from a chromatogram: open a chromatogram, define a report style in which the Calibration curve object is defined in the corresponding part of its method, and then click on the icon.
- Printing from a calibration curve by clicking on the icon.

Glossary

External standard: The external standard calibration allows calculation of the identified peak quantities, using a calibration curve or a manual response factor, which is entered by the user.

CompassCDS Configuration Manager: It is CompassCDS maintenance manager. It allows the user to declare, configure, manage chromatographic systems, and define the user base (users, groups, projects, profiles).

CompassCDS Report Editor: It is the report printing manager of CompassCDS.

Internal standard: Internal standard calibration requires the addition of a known quantity of defined compound(s) in every sample to be analyzed. In the same way as for the external standard, a calibration curve is created or manual response factors entered. The calibration curve created takes into account the internal standard quantity associated with the compound. This calculation method is used more in gas chromatography to compensate for the inaccuracy of the injection volume (manual injection).

Method templates: The method templates are models for new methods (not compulsorily defined on the same system). For reusing variables, chromatograms or peak report formats, etc. with other methods, save the current method as a template which you can then use to create a new method. The method template uses the entire method, except the instrument control section.

Popup menu: A popup menu is a menu associated with an object and hidden most of the time. To view the popup menu of an object, position the cursor inside the object and press the right mouse button. Then choose any item of the popup menu with the left mouse button. The object can be a curve, a table, a browser, etc.

Standalone: This term concerns the configuration mode of the software. It means that the software is not set for a network configuration, but is used locally on one computer.

System variables: Many variables allowing for specific calculations on peaks, groups or global chromatogram are available in CompassCDS. These variables are calculated automatically for each chromatogram.

User input variables: As opposed to a system variable, a user input is created by the user. Two user input types exist: the user input for which user must then enter a value or text and the user formula for which the user creates customized calculations, not made by default in CompassCDS.

Workstation: It is the name of the computer on which the software is installed.

See also the CompassCDS Configuration Manager User Guide Glossary.

CompassCDS
Photodiode Array Software
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501610
Revision B

Contents

Introduction 3
General 3
PDA Features 3
Acquisition and baseline monitoring 3
Purity calculations 3
Getting Started 4
Configuring the System 4
Starting an Acquisition 4
Building a Method 4
Defining Method Parameters 4
Starting an Acquisition 5
How to View an Acquisition 5
Viewing an Acquisition 5
Viewing a Chromatogram 7
Application Details 8
PDA Data Structure 8
PDA Method and Acquisition 9
The 3D Method 9
The PDA Sub Method 10
The Report Sub Method 11
The Extracted Chromatogram Method 12
The 2D-Signal Chromatogram Method 12
The PDA Specific Variables 12
Baseline Monitoring and Acquisition 14
Following Acquisition 14
First tab (System name + PDA): 15
The Acquisition View Pop-up Menus 17
The Acquisition View Properties 20
Displaying PDA Data 25
Opening a 3-D Chromatographic Data File 25
PDA Chromatogram Display Mode 26
Modifying the display properties 29
The 3D View 34
Displaying Chromatograms and Spectra 36
Getting Chromatograms and Spectra 36
The ASCII Export of Spectra 37
The Spectra Report Editor 38
PDA Data Processing 41
The Spectral Library Editor 41
The ASCII Import of Spectra 44
The CompassCDS ASCII format of spectra 44
The Spectral Library Report Editor 45
The Library Search 48
The Manual Search 48
The Peak Purity 54
The Matching Algorithms of CompassCDS 60
The Spectrum Calculator 61
Reprocess the PDA Chromatogram 62
Index 65

Introduction

General

In conventional HPLC, acquisition of a single chromatogram monitored at a certain wavelength may include many unresolved peaks.

The use of a photodiode array detector adds a third dimension to the chromatogram: the wavelength. The PDA application is a part of the standard CompassCDS Software. In addition to the classical features, the PDA part of CompassCDS is designed to handle this more complex data structure and allows you specific treatment such as:

- determining the optimal wavelength for each peak,
- doing a qualitative analysis using a library search,
- calculating peak purity.

PDA Features

Acquisition and baseline monitoring

- Data display during acquisition and already acquired data display. The 3D data is displayed in real time during the acquisition.
- Qualitative analysis

Purity calculations

- Spectral Comparison at different peak widths
- Spectral Comparison for all points of the peak
- Identification by a library search
- Report display and print

You will rapidly adapt to the PDA environment: in addition to the classical menu at the top of the screen, there are also pop-up menus inside your chromatogram, your spectrum, your isocurve, and your 3D view.

Getting Started

Configuring the System

First, you must create a system in the configuration manager (CompassCDS Configuration Manager). Refer to the CompassCDS Configuration Manager User Guide to create your system.

Starting an Acquisition

Building a Method

In the menu, select ***FILE / NEW / NEW METHOD***.

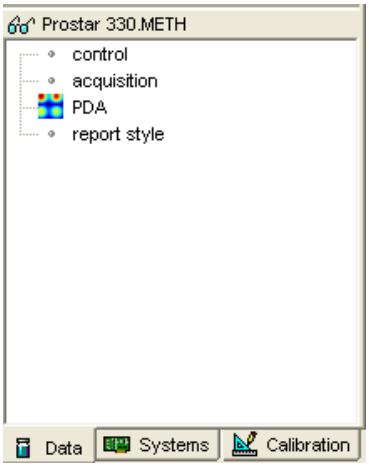
Select the project in which the method will be used (if in all project mode) and the chromatograph on which it will be applied.

Press *Next.*

Enter the name of the method, and optionally, a text description of the method which may also be entered and will appear as a comment in the Open File window.

The method is opened with default parameters in CompassCDS.

To display the parts of the 3D-method, click on the corresponding item in the browser. The parts of the method appear:



Click on the parts of this method to edit the parameters in the right part of the screen.

Defining Method Parameters

In the browser, click on *Control*.

Enter the required instrument method parameters. Refer to the instrument User Guide for more details.

In the browser, click on *Acquisition*.

In this section, parameters may be set that will appear by default in the acquisition windows. For example, the run name can be entered (the identifier or suffix will be implemented automatically for each run).

In the browser, click on *PDA.*

In this section, wavelengths can be defined to automatically extract chromatograms at the end of the run. A sub section corresponding to the chromatogram is automatically added. Processing parameters for each extracted chromatogram can now be defined.

Save the method by using the pull-down menu selections ***FILE / SAVE / SAVE METHOD***, or by clicking on the *Save Method* icon, or by pressing the key combination Shift+Ctrl+2.

Starting an Acquisition

Before starting a baseline monitoring or an acquisition, a method must be prepared for the corresponding system (chromatograph).

It is possible to launch a Quick Start (only one acquisition) or a Sequence of acquisitions. Refer to the CompassCDS User Guide to learn how to start an acquisition.

How to View an Acquisition

Viewing an Acquisition

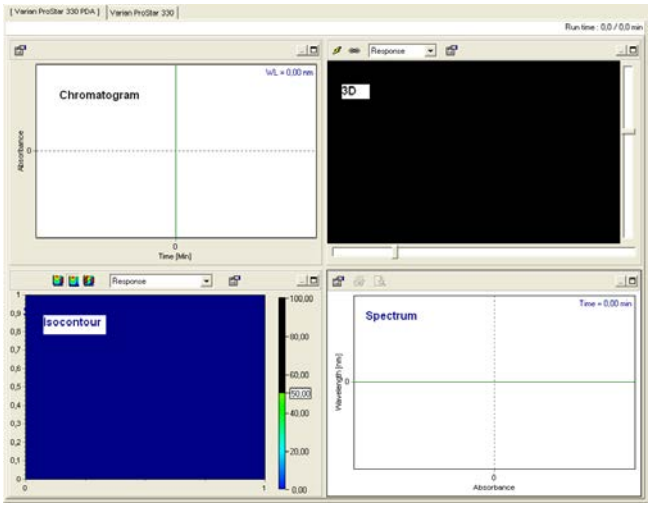
In the CompassCDS main screen, go to the Systems tab.

In the browser, select the system where the sample was injected. Check *PDA* to view the 3D data acquisition. Check *status* to also view the system status. Possibly, check *Chromatogram* to view the 2D signal if any.

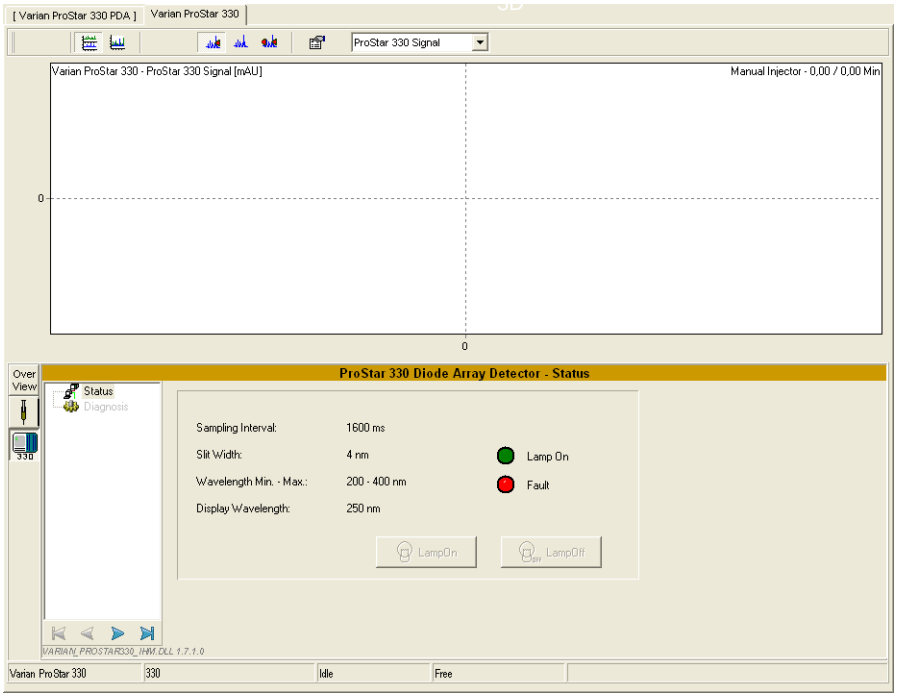
In the right part of the screen, two tabs appear.

The first one, named PDA (preceded by the system name) is composed of 4 views:

- the Chromatogram view
- the 3D view (which is initially empty)
- the Isocontour plot view
- the Spectrum view



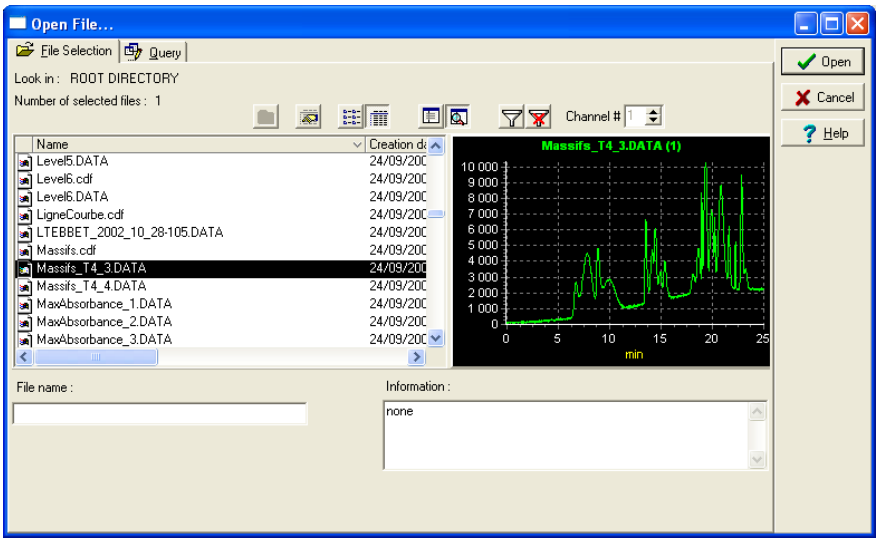
The second tab, named by the system name, contains the system status and possibly the 2D signal(s).



Viewing a Chromatogram

Once the chromatogram has been acquired, open and process it press .

The Open File window appears:

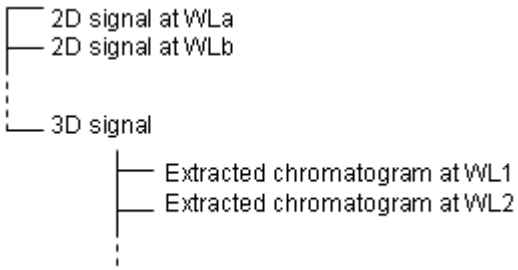


In this window, use the scroll bars to scroll down the list and click on the just acquired chromatogram. Alternately, type the first few letters of the chromatogram name in the file name box and only the chromatograms whose names begin with these letters will be displayed.

Application Details

PDA Data Structure

By default, PDA data consist in one 3D signal and possibly one or several chromatograms (2D signal) acquired at fixed wavelength. Chromatograms can additionally be extracted from the 3D signal. Data structure is as follows:



The 2D signals can be processed as classic chromatograms (integration, peak and group identification, calibration, etc.). From the 3D signal, user can add spectra in libraries or perform manual library search. From the extracted chromatograms, the user can perform all the classical processing of 2D channels and can also calculate peak purity or perform automatic library search.

PDA Method and Acquisition

To launch an acquisition the user must first define a 3D method and optionally, extract chromatogram methods for having chromatograms automatically extracted at the end of the run.

The 3D Method

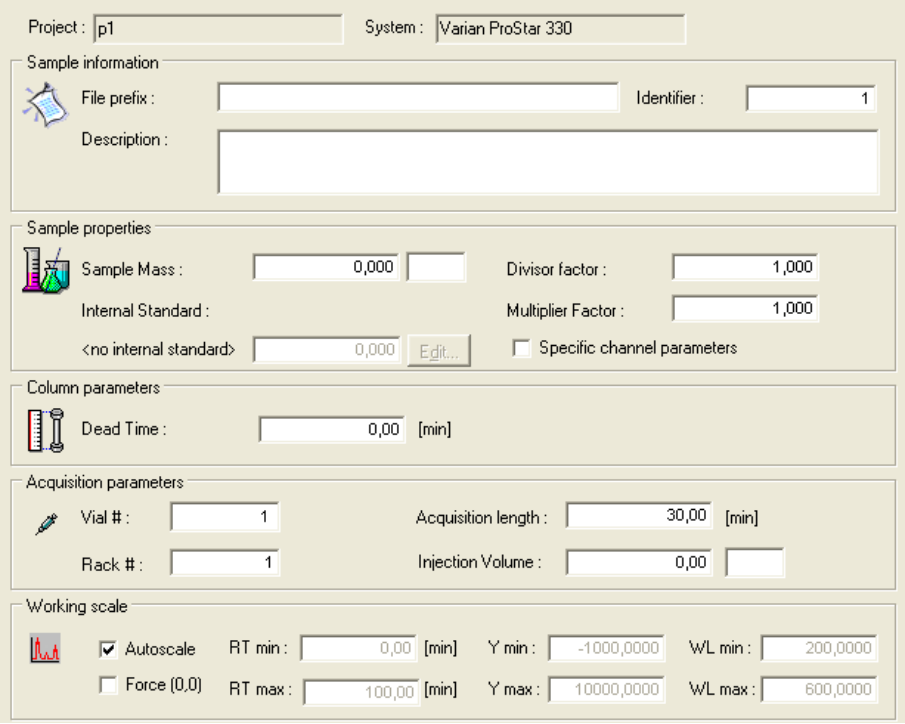
The 3D-method is divided into four parts.

The Control Sub Method

This part of the method depends on the instrument connected to the channel. The control method is composed of all the parameters that can be set for this instrument. Refer to the instrument driver manuals to learn how to fill this section.

The Acquisition Sub Method

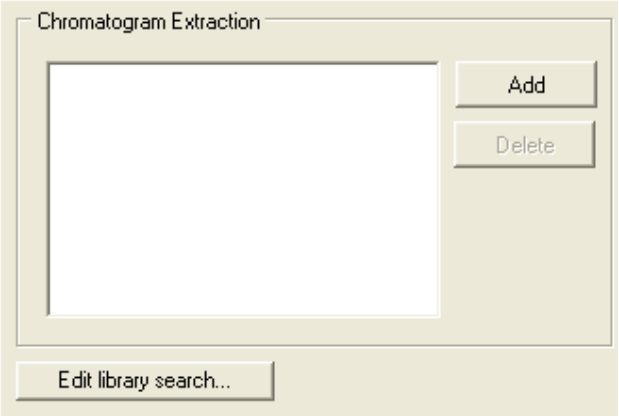
In the acquisition method, default parameters can be set. They will be displayed in the acquisition windows: Quick Start or Sequence.



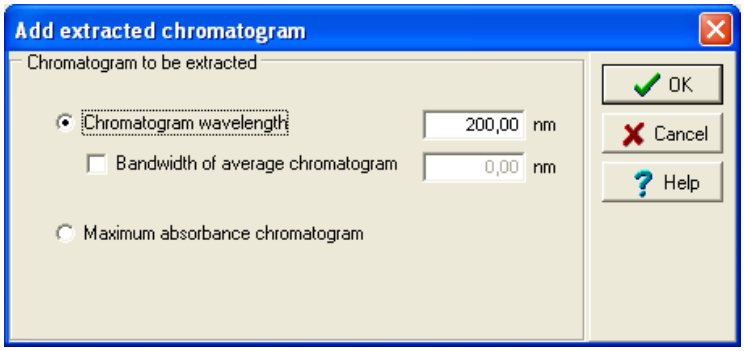
It is possible to modify these parameters before starting the acquisition. Refer to the CompassCDS User Guide for a description of the fields.

The PDA Sub Method

This sub section allows you to select the chromatograms automatically extracted at the end of the acquisition and to define the parameters of automatic library search. The library search is also described on page 48. The following screen is displayed when the PDA sub method is checked.



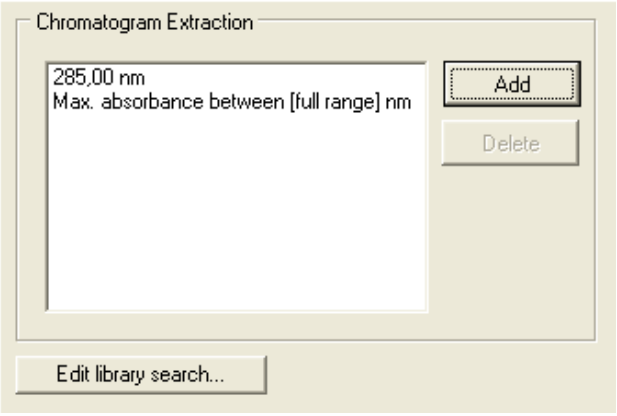
In the Chromatogram Extraction field, you can **add** the chromatogram you want to automatically extract after the acquisition. Click on the *Add* button, to choose the chromatogram you want to extract. The following screen appears:



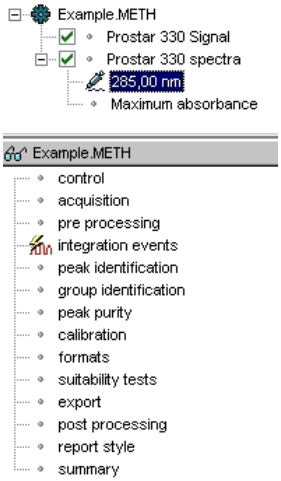
You can choose to extract a chromatogram at either a given wavelength or at an average wavelength over a defined bandwidth, or at the maximum absorbance chromatogram obtained on the full acquisition wavelength range or in a user defined wavelength range.

The maximum absorbance curve is a virtual chromatogram where the wavelengths are chosen so that each chromatogram point is plotted at the optimum wavelength which gives the maximum absorbance.

The following screen gives an example of the extraction of the chromatogram at 285 nm and the maximum absorbance chromatogram.



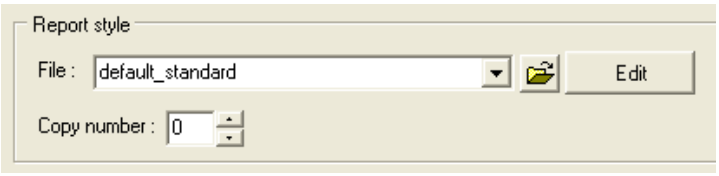
For each extracted chromatogram, a sub-section is created in the browser. Its name corresponds to the wavelength at which the chromatogram is extracted:



An acquisition can be started without specifying an extracted chromatogram.

The Report Sub Method

The **Report Style** sub section allows you to define the PDA report style. The following screen is displayed:



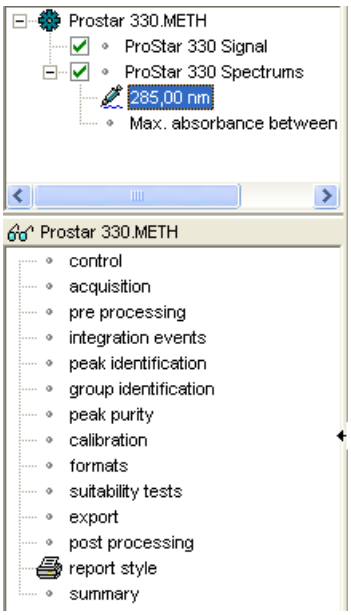
In the **File** box, select the name of the report style to be printed. Styles should first be created in CompassCDS Report Editor (see the corresponding User Guide).

To look at the selected report, press the *Edit* button: the CompassCDS Report Editor is opened and displays the report style.

To print automatically one report after an acquisition, enter 1 in the **copy number** box. If 0 is selected, no printing will be done.

The Extracted Chromatogram Method

A method sub-section is created for each extracted chromatogram. Check the right channel in the browser to modify or display the corresponding method. For example, in the following screen, the method displayed in the browser is the method of the chromatogram extracted at 285 nm.



The **Control** and the **Acquisition** part are the same for the 3D data and for the extracted chromatogram(s).

All the sub parts of the extracted chromatogram(s) are described in details in the CompassCDS User Guide, except the peak purity one.

The peak purity part is described on page 54.

The 2D-Signal Chromatogram Method

The 2D-signal chromatogram method can be handled as a classical method. See the CompassCDS User Guide for a detailed explanation for each method sub-part.

The PDA Specific Variables

CompassCDS PDA incorporates many standard variables that can perform calculations on the entire sample.

It is also possible to define custom variables for calculations that not already belong to the default CompassCDS variables such as:

> “user input”: variables for which the user must enter a value or a text.
>
> “user formula”: variables that allow CompassCDS non default calculations (see the CompassCDS User Guide for more details).

All the PDA-variables (system, user input and user formula) are defined using specific parameters, described in the CompassCDS User Guide.

Most of the Variables present by default in CompassCDS PDA are the same as the ones present in CompassCDS. Only the PDA specific variables are described here. Please refer to the CompassCDS User Guide to have a complete description of other variables.

Variables of the 3D Channel

Only one 3D variable is PDA specific. It is a global variable:

> **Number of WL Points [NWLPOINTS]**: Number of points acquired in the UV spectrum.

Note: The global variables belong to the chromatogram in its whole. The global variables can be displayed in the chromatogram properties. Select the menu options *DATA / CHROMATOGRAM PROPERTIES* in the main menu or press the icon.

Variables of the 2D-signal Channel

No specific PDA variables exist. (refer to the CompassCDS User Guide for more details).

Variables of the Extracted Chromatogram

PDA specific variables exist by default in CompassCDS PDA related to purity and search in library. All these variables are Peak variables.

Note: The peak variables can be displayed in the peak report. (Choose REPORT PROPERTIES in the popup menu and select the variables for report display).

Purity Variables

Area Impure (%) [AREA_IMPURE]: Area percentage of peak computed as impure. Only computed if the purity is calculated for "all spectra" of each peak (see page 54).

Area Medium (%) [AREA_MEDIUM]: Area percentage of peak computed as medium. Only computed if the purity is calculated for all spectra of each peak.

Area Pure (%) [AREA_PURE]: Area percentage of peak computed as pure. Only computed if the purity is calculated for "all spectra" of each peak (see page 54).

Pur(Apex) [PURITY_APEX]: Purity value calculated at peak apex. Computed for all options of spectral purity (see page 54).

Pur(FBL) [PURITY_FB]: Purity value calculated at peak front baseline. Computed for all options of spectral purity except "3 spectra" and "apex only" (see page 54).

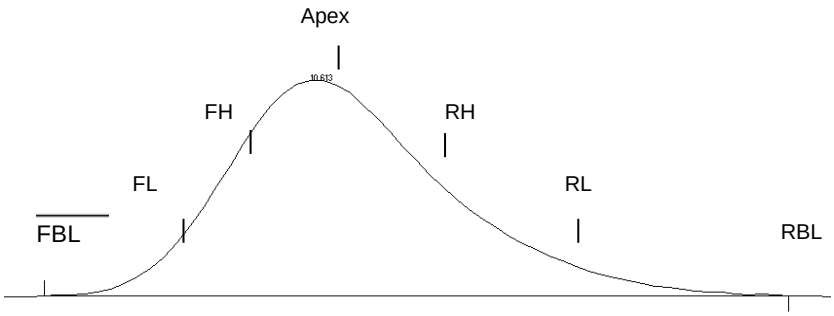
Pur(FH) [PURITY_FH]: Purity value calculated at a peak height defined by the user. Four heights maximum can be defined. This is the front high value. Computed for all options of spectral purity except "apex only" (see page 54).

Pur(FL) [PURITY_FL]: Purity value calculated at a peak height defined by the user. Four heights maximum can be defined. This is the front low value. Computed for all options of spectral purity except "3 spectra" and "apex only" (see page 54).

Pur(RBL) [PURITY_RB]: Purity value calculated at peak rear baseline. Computed for all options of spectral purity except "3 spectra" and "apex only" (see page 54).

Pur(RH) [PURITY_RH]: Purity value calculated at a peak height defined by the user. Four heights maximum can be defined. This is the rear high value. Computed for all options of spectral purity except "apex only" (see page 54).

Pur(RL) [PURITY_RL]: Purity value calculated at a peak height defined by the user. Four heights maximum can be defined. This is the rear low value. Computed for all options of spectral purity except "3 spectra" and "apex only" (see page 54).



Search in Libraries Variables

Matching Component [MATCHCOMPO]: name of the component which better matches the unknown spectra.

Matching Factor [MATCHFACTOR]: matching factor corresponding to the component which better matches the unknown spectra.

Matching Library [MATCHLIBRARY]: Spectra library of the component which better matches the unknown spectra.

Others

WL(MaxAbs) [WL_MAXABS]: wavelength at the maximum absorbance of the peak.

Baseline Monitoring and Acquisition

Before starting a baseline monitoring or an acquisition (Quick Start or sequence), a 3D-method must be prepared for the corresponding system (chromatograph).

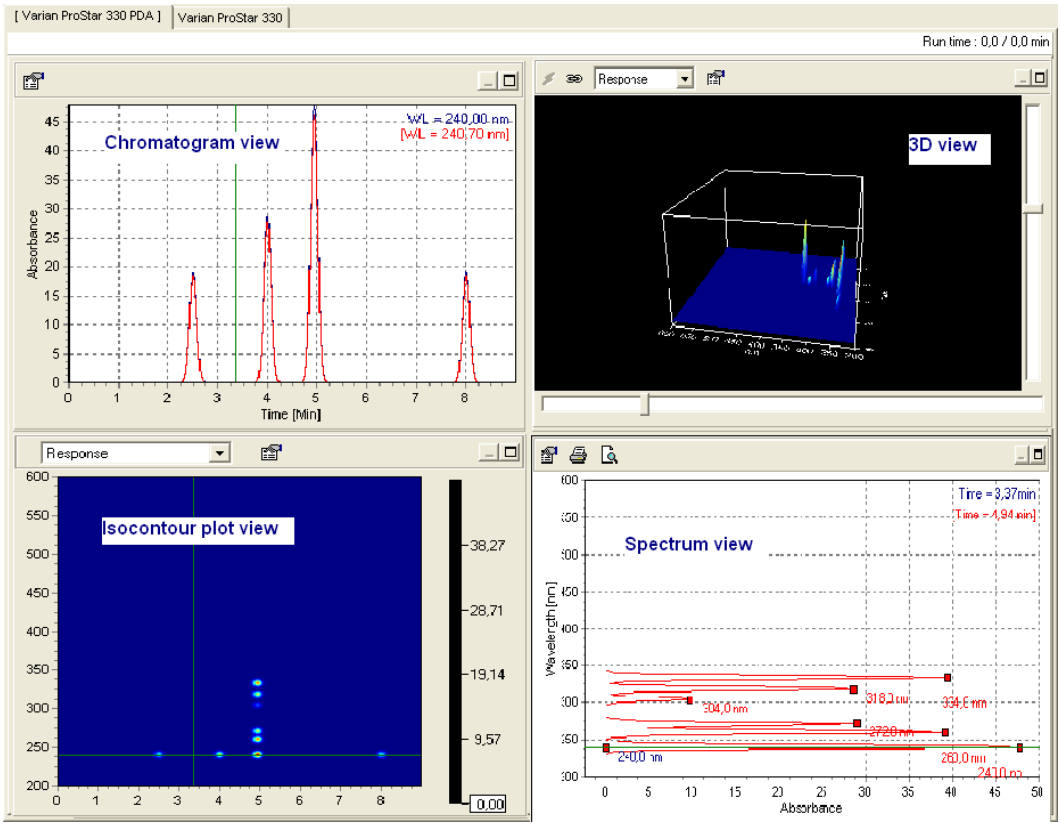
See the CompassCDS User Guide on how to launch a baseline monitoring, a Quick Start (injection of one sample) or a sequence (injection of several samples).

Following Acquisition

To look at a PDA chromatogram during its acquisition, select the **Systems** tab. All the systems defined in the project in which the user is connected, are listed in the browser.

If a PDA system name is checked, two tabs are created: one named by the system name following with PDA, the other named by the system name only.

First tab (System name + PDA):



By default, the screen is composed of four parts:

- the Chromatogram view
- the 3D view (which is initially empty)
- the Isocontour plot view
- the Spectrum view

Use the following icons or the scrolling list to:

Stop the current run. If the instrument is fully controlled, CompassCDS does not receive any information that the instrument is stopped. It is therefore necessary to stop the run within the software. CompassCDS will ask for a confirmation before stopping a run. Only the person who started an acquisition, or those users defined in the CompassCDS Configuration manager have the right to stop it. In the case of double injection acquisition, user can choose to stop either one or both acquisitions.

Modify the acquisition time. Note that by decreasing the acquisition time to a value less than the current run time, the acquisition will be stopped.

Display the views with automatic scaling: the scales are updated after each acquisition point, so the entire chromatogram is displayed.

Display the views in a fixed window. The parameters can be changed in the properties.

Set the parameters for the x-scale that moves along as the acquisition runs. For example, it is possible to view only the last minute of acquisition. To modify the width of this window, use the properties (see the corresponding icon just below) and in the scrolling section, it is possible to change this default value.

Modify the acquisition view properties, see page 20.

Select which response you want to display. This scrolling list is present in both isocontour map and 3D view. Four choices are proposed: Response, Threshold up, Threshold down and Threshold between to display respectively all the absorbance levels with the same importance or emphasize certain ones. All absorbances inferior to the lower limit or superior to the upper limit will have the same color.

Create the 3D view. By default, the 3D view is empty.

Synchronize the zoom between the views.

Maximize the corresponding view to display it in the full area dedicated to acquisition views

Minimize the corresponding view size and return in the 4 views mode.

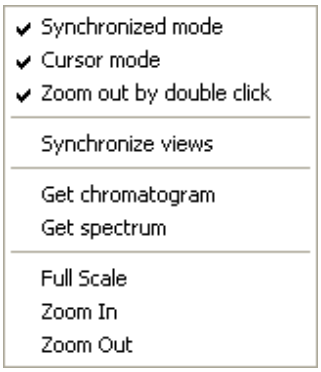
Print a spectra report

Print preview a spectra report

The Acquisition View Pop-up Menus

In each of the views, pop-up menus accessible by mouse right-click provide access to multiple functions.

The Isocontour Plots View Pop-up Menu



If the **Synchronized mode** is checked, the views are always synchronized: zoom done in one view is always applied in other views.

If the **Cursor mode** is checked, when you move the cursor using the mouse in the isoabsorbance map, the corresponding chromatogram and spectrum are displayed in the corresponding views. The time and wavelength position markers are moved accordingly in each view. When a point is correctly chosen, you can deactivate the cursor mode (by unchecking it in the pop-up menu). The chromatogram and the spectrum do not change regardless of the mouse movement in the isocontour map except after a left mouse double-click.

If **Zoom out by double click** is checked, the last zoom is applied after each double clicks.

Click on the **Synchronize views** to apply punctually the same zoom in all the views if synchronized mode is unchecked.

Click on the **Get chromatogram** option to fix one chromatogram at the current wavelength.

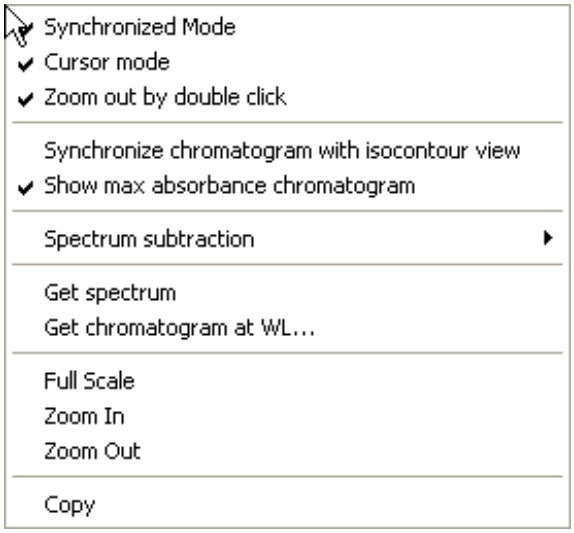
Click on the **Get spectrum** option to fix one spectrum at the current time.

Click on **Full Scale** to return to the full scale.

Click on **Zoom In** to magnify the view.

Click on **Zoom Out** to reduce the view.

The Chromatogram View Pop-up Menu



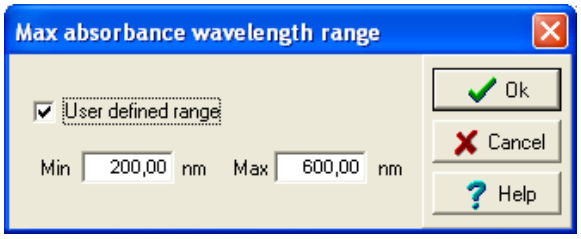
If the **Synchronized mode** is checked, the views are always synchronized: zoom done in one view is always applied in other views.

If the **Cursor mode** is checked, when you move the cursor in the views using the mouse, the time position marker is moved in the chromatogram and isocontour views and the corresponding spectrum is displayed in the spectrum view. When a point is correctly chosen, you can deactivate the cursor mode (by unchecking it in the pop-up menu). The time repair does not move and the spectrum does not change regardless of the mouse movement in the chromatogram view except after a left mouse double click.

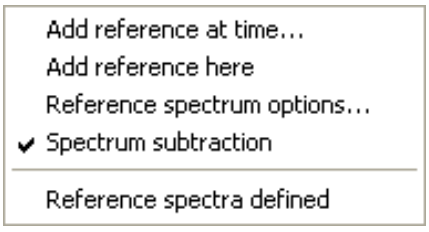
If **Zoom out by double click** is checked, the last zoom is applied after each double clicks.

Click on the **Synchronize chromatogram with isocontour view** option to punctually apply the isocontour view zoom on the chromatogram when synchronized mode is unchecked.

Click on **Show max absorbance chromatogram** to display the maximum absorbance chromatogram which shows all components at their maximum absorbance. The following screen appears:



Click on the **Spectrum subtraction** option to select a spectrum to subtract. The following screen appears:



Choose **Add reference at Time** and enter manually a time where a reference spectrum will be defined in the appearing screen.

Click on **Add reference here** to define a reference spectrum at the cursor time.

Choose **reference spectrum options** to remove some reference spectra.

Check **Spectrum subtraction** to activate or not the subtraction. A spectrum is interpolated between two consecutive reference spectra and subtracted to all spectra of the corresponding interval. The results of the subtraction are given in the spectrum view.

When reference spectra have been defined, "Reference spectra defined" appears in the bottom part of that popup menu. Else, "No reference spectrum defined" appears.

Click on **Get Spectrum** to fix one spectrum at the current time.

Click on **Get Chromatogram at WL** to enter manually a wavelength and get the corresponding chromatogram.

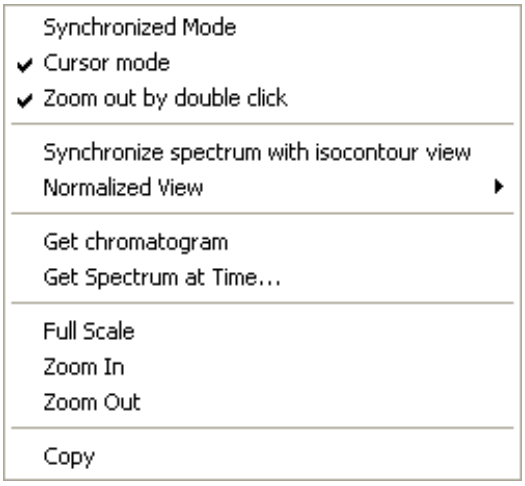
Click on **Full Scale** to return to the full scale.

Click on **Zoom In** to magnify the view.

Click on **Zoom Out** to reduce the view.

Click on **Copy** to copy the chromatogram as displayed and paste it to another application.

The Spectrum View Pop-up Menu



If the **Synchronized mode** is checked, the views are always synchronized: zoom done in one view is always applied in other views.

If the **Cursor mode** is checked, when you move the cursor in the view using the mouse, the wavelength position marker is moved and the corresponding chromatogram is displayed in the corresponding view. When a point is correctly chosen, you can deactivate the cursor mode (by unchecking it in the pop-up menu). The wavelength marker and the corresponding chromatogram the do not change whatever the mouse movement in the spectrum view except after a left-mouse double click.

If **Zoom out by double click** is checked, the last zoom is applied after each double click.

Click on **Synchronize with isocontour view** to punctually apply the isocontour view zoom on the spectrum when synchronized mode is unchecked.

Click on **Normalized View** to apply a specific scale on the absorbance axis. A submenu is displayed with two choices (**auto** and **at WL**). Depending upon the chosen option, the spectra are zoomed in such a way that the signal corresponding to the maximum

absorbance (auto mode) or the absorbance at the specified wavelength (at WL mode) represents 5 to 95% of the absorbance axis.

Click on the **Get chromatogram** option to fix one chromatogram at the current wavelength.

Click on **Get spectrum at time** to enter manually a time and get the corresponding spectrum.

Click on **Full Scale** to return to the full scale.

Click on **Zoom In** to magnify the view.

Click on **Zoom Out** to reduce the view.

Click on **Copy** to copy the chromatogram as displayed and paste it to another application.

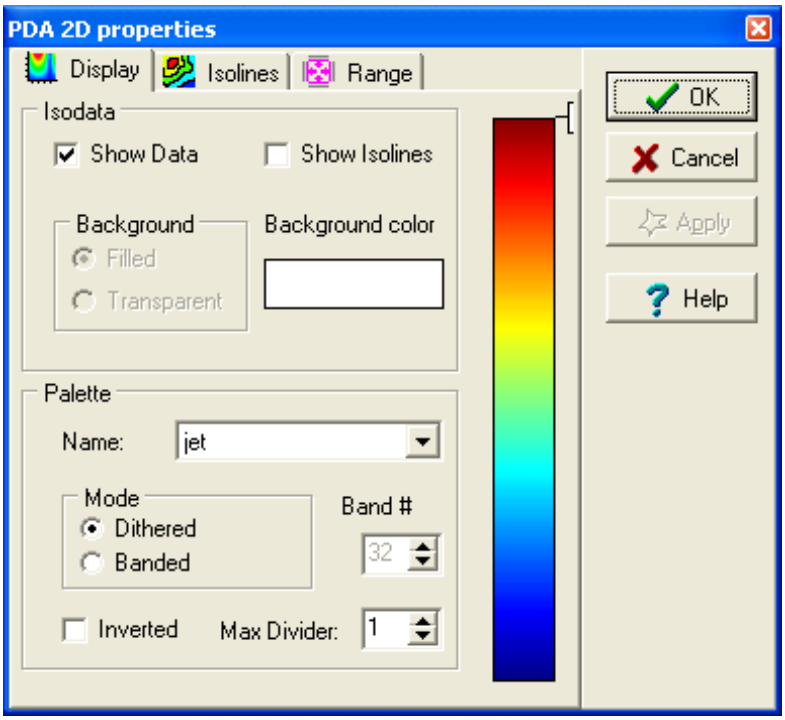
The Acquisition View Properties

Click on the button in each view to change its display properties.

The Isocontour View Properties

Three tabs allow you to modify the acquisition displaying properties: Display, Isolines and Range.

Display



In this tab customize the isocontour view display.

Check or uncheck **show data** to display or hide the acquisition points when *show isolines* is checked. If **show data** is unchecked, only the isolines are displayed.

Check or uncheck **show isolines** to display or hide the isolines.

If *show data* is unchecked, you can change the background color. Click on the mouse left button in the **background color** field and choose a color in the appearing screen. It is also possible to make the background transparent and display the scale grid (select **transparent** in the background field).

In the **palette** field customize the color scale of the view. The resulting scale is displayed on the screen right column. Change the **name** to modify the absorbance-color correspondence. It is also possible to invert the scale (check **inverted**) or to emphasize certain absorbances by changing the value of the **Max Divider** (see below for more explanation). The coloration can also be **dithered** or **banded**. In this case you can choose the number of bands.

What does the Max Divider Parameter mean?

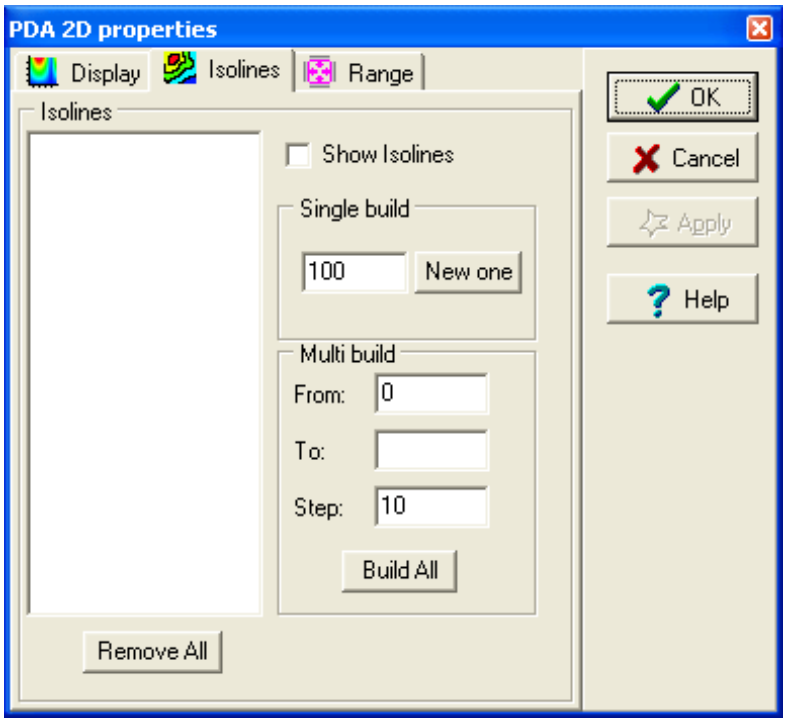
The Max Divider Parameter will define the limit of color levels displaying the isocontour view.

The inferior limit of the color level 7 (level for the largest absorbance values) will be divided by the max divider parameter. As a consequence, if Max Divider is superior to one, this level range will be larger and will contain more data points: above a certain value of absorbance, the data will be displayed with the same color (the color chosen for level 7).

The other color level range (1 to 6) will be narrowest. As a consequence, the small variations will be emphasized on the isocontour view.

As a conclusion, if you want to emphasize the small variations of the isocontour view, choose a large value.

Isolines



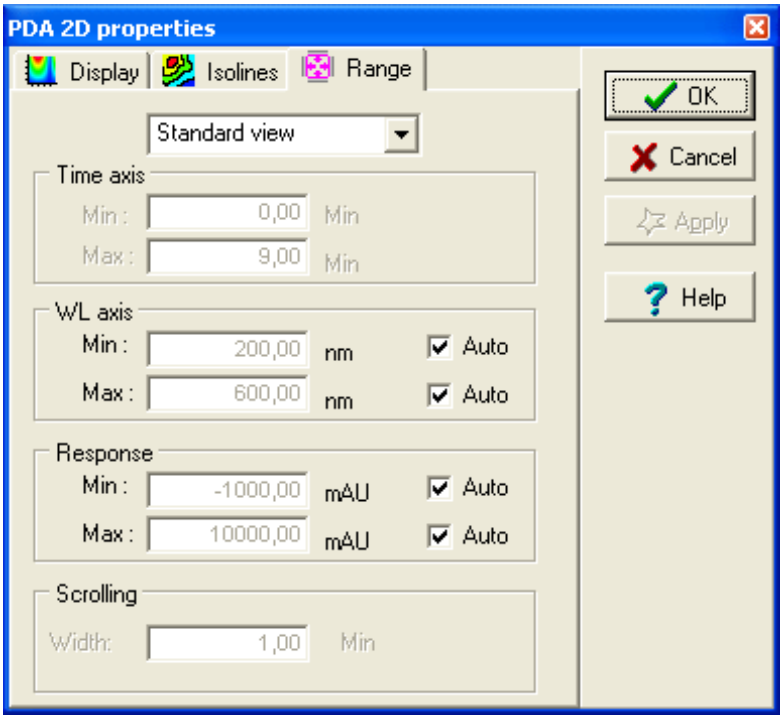
In the **Isoline** tab, check **Show Isolines** if you want to display isolines.

Choose the absorbance line you want to display in the single build field and then click on *New one.*

To automatically build the isolines, choose in the **Multi build** field, the minimum absorbance (From: field), the maximum absorbance (To: field) and the Step. Then click on *Build All.*

After choosing the isolines, their absorbance values are given in the Isolines field. You can uncheck the isolines you do not want to display.

Range

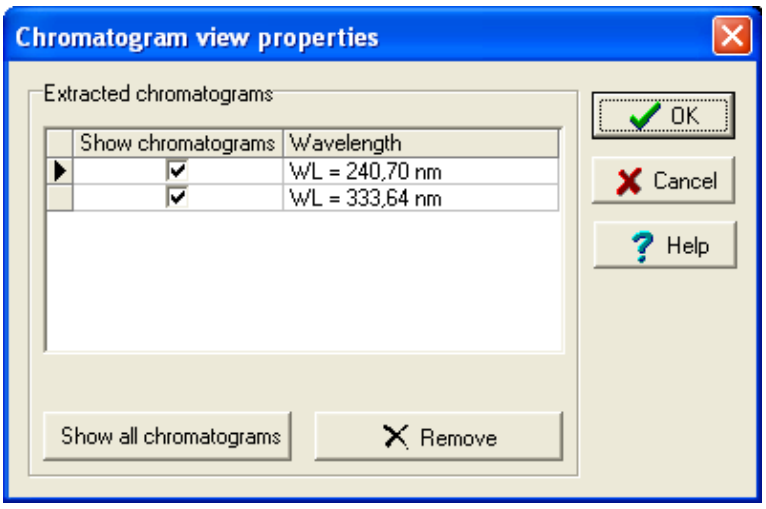


In the **Range** tab, you can choose the acquisition view properties (standard, fixed, or scrolling view) using the scrolling list. If the standard view is chosen, you can modify the Wavelength and the Response axis range. If the fixed view is chosen, moreover, the Time axis range can be modified. If the scrolling view is chosen, the scrolling width must be fixed in the field.

An automatic scale means that the minimum is set to the minimum signal value and the maximum is set to the maximum signal value: the response and the WL-scale are large enough to display all the acquisition points.

The Chromatogram View Properties

The chromatogram view properties allows the user to manage the chromatogram to display. The screen looks as follows:



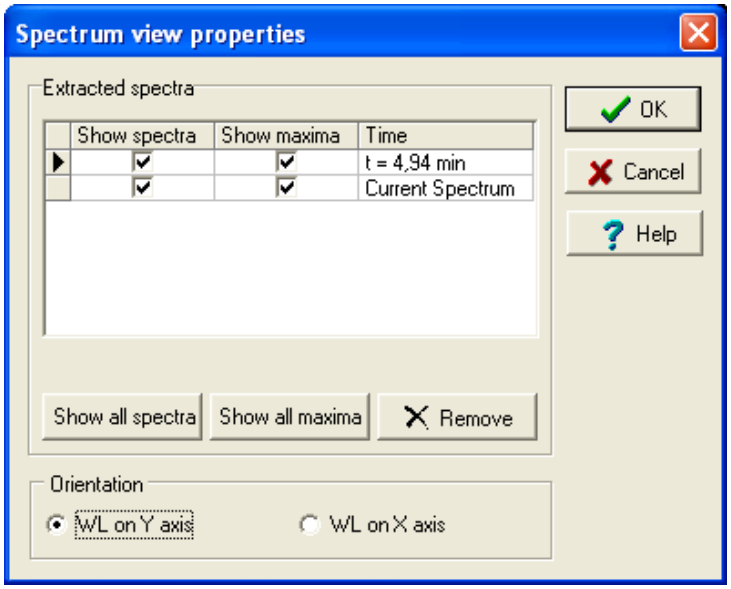
Choose which chromatogram(s) you want to display by checking the corresponding box.

Press the *Remove* button to delete chromatogram(s) you do not want to display.

Press the *Show all chromatograms* button to display all the listed chromatograms.

The Spectrum View Properties

The spectrum view properties allow you to manage the spectra to display. The screen looks as follows:



Choose which spectrum(a) you want to display by checking the corresponding box in the *Show spectra* column.

Choose which spectrum maximum(a) you want to display by checking the corresponding box in the *Show maxima* column. You can also choose to hide/show given maximum(a) by clicking on their box directly in the spectrum view.

Press the *Show all spectra* button to display all the listed spectra.

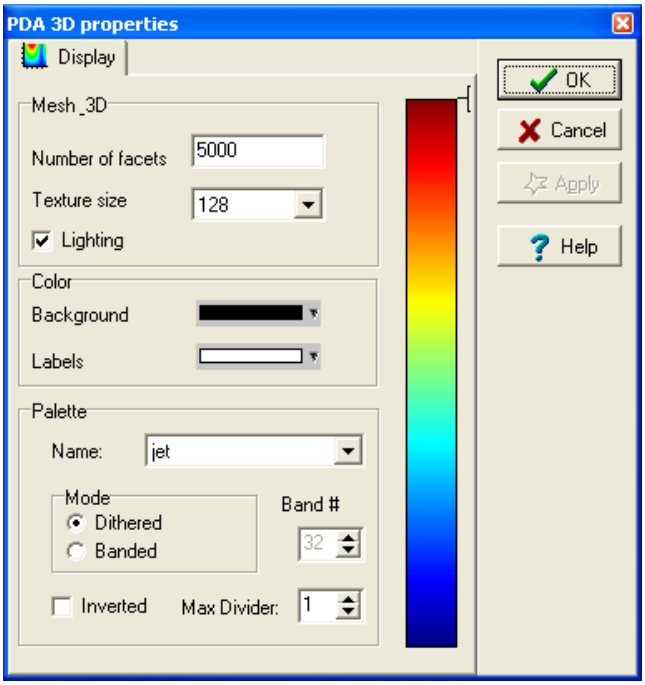
Press the *Show all maxima* button to display the maxima of all the selected spectra.

Press the *Remove* button to delete spectrum(a) you do not want to display.

Select the *WL on Y axis* or *WL on X axis option* to display the spectrum vertically or horizontally.

The 3D View Properties

The following screen allows you to modify the acquisition 3D displaying properties:



You can modify the appearance of the 3D object:

The number of facets and the texture size can be modified in the Mesh-3D field.

The color of the background and the labels can be chosen in the color field.

In the **palette** field customize the color scale of the view. The resulting scale is displayed on the screen right column. Change the **name** to modify the absorbance-color correspondence. It is also possible to invert the scale (check **inverted**) or to emphasize certain absorbance by changing the value of the **Max Divider** (see below for more explanation). The coloration can also be **dithered** or **banded**. In this case you can choose the number of bands.

What does the Max Divider Parameter mean?

The Max Divider Parameter will define the limit of color levels displaying the 3D view.

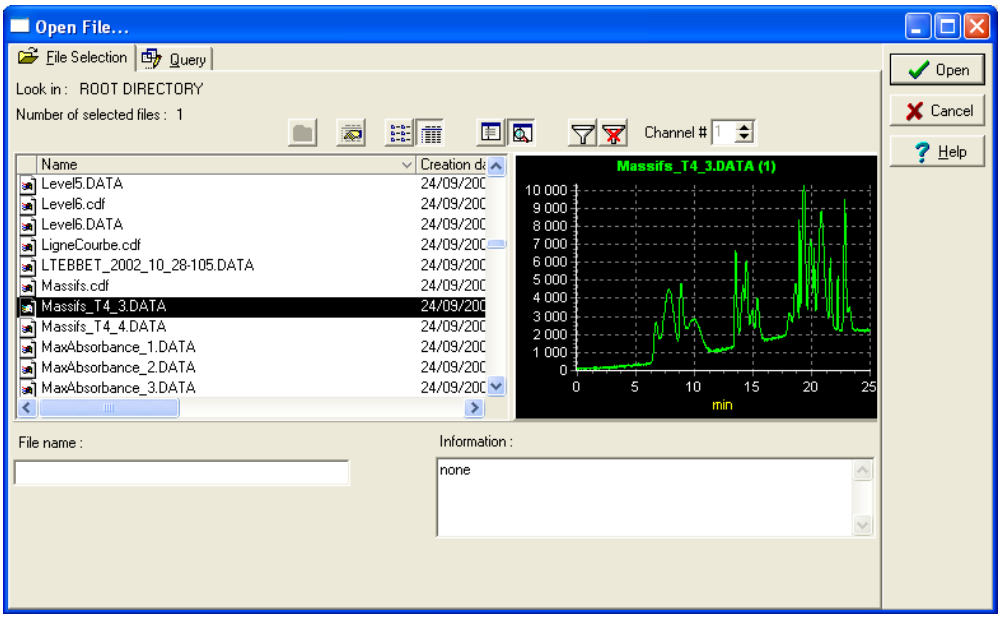
The inferior limit of the color level 7 (level for the largest absorbance values) will be divided by the max divider parameter. As a consequence, if Max Divider is superior to one, this level range will be larger and will contain more data points: above a certain value of absorbance, the data will be displayed with the same color (the color chosen for level 7).

The other color level range (1 to 6) will be narrowest. As a consequence, the small variations will be emphasized on the 3D View. As a conclusion, if you want to emphasize the small variations of the 3D display, choose a large value.

Displaying PDA Data

Opening a 3-D Chromatographic Data File

Select ***FILE / OPEN / OPEN CHROMATOGRAM*** or click on the button or press Ctrl+O. When the Open File dialog box appears, select your file in the File selection tab. Double click on it or select OK. No preview is displayed for the spectrum channel in the right part of the Open File box for PDA chromatograms.

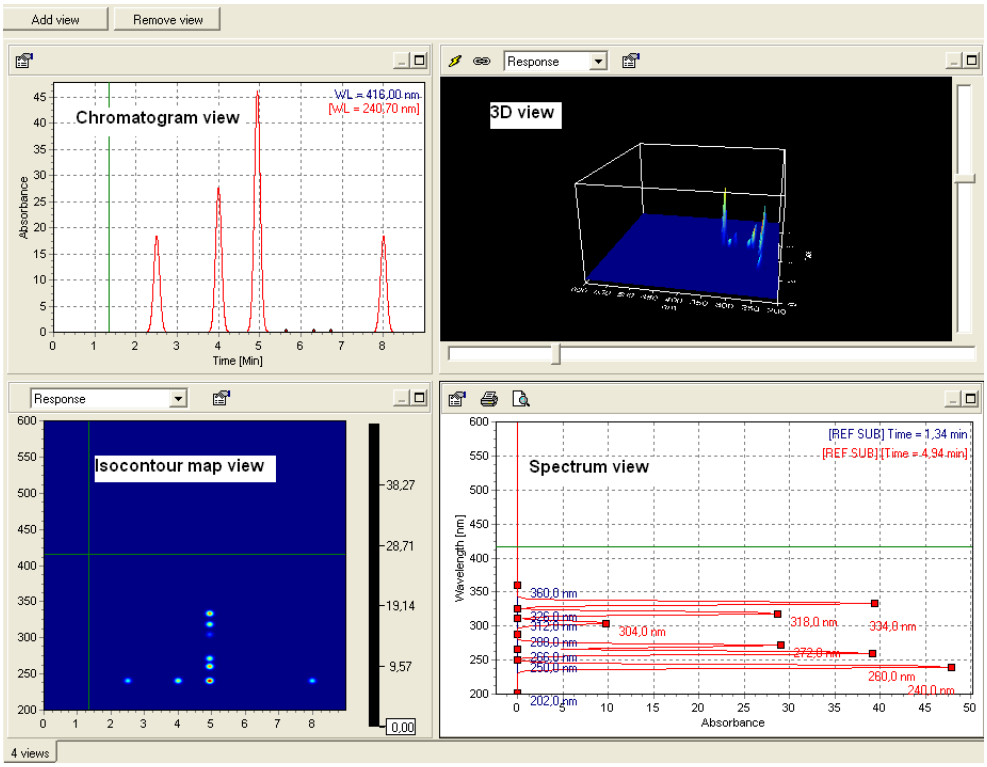


See the CompassCDS User Guide to know how to manage the open file box.

PDA Chromatogram Display Mode

In CompassCDS, four standard display modes exist named '4 views', '3 views', '3D only' and 'Spectral extraction'.

By default, when a PDA chromatogram is opened, the ‘4 views’ is displayed in the right part of the screen and the following screen appears:



The ‘4 views’ consists of:

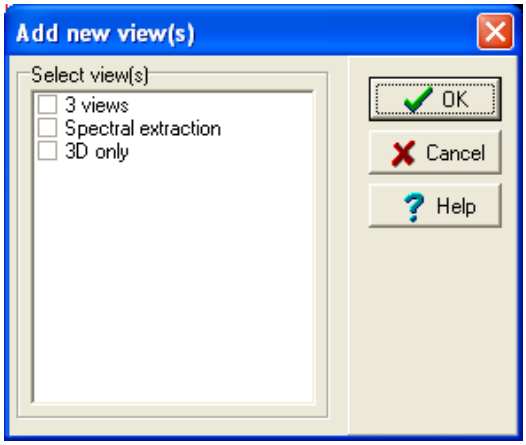
The isocontour view: 3D data displayed in a 2D view. The absorbance levels are represented by different colors, each color corresponding to an absorbance range.

- The 3D view.
- The chromatogram view.
- The spectrum view.

The chromatograms and the spectra displayed correspond to the current cursor position in the isocontour map and user defined chromatograms and spectra (see page 36 for details).

You can add several other views using the Add view button or delete the opened ones using the Remove view button.

When you click on Add view, the following screen appears:

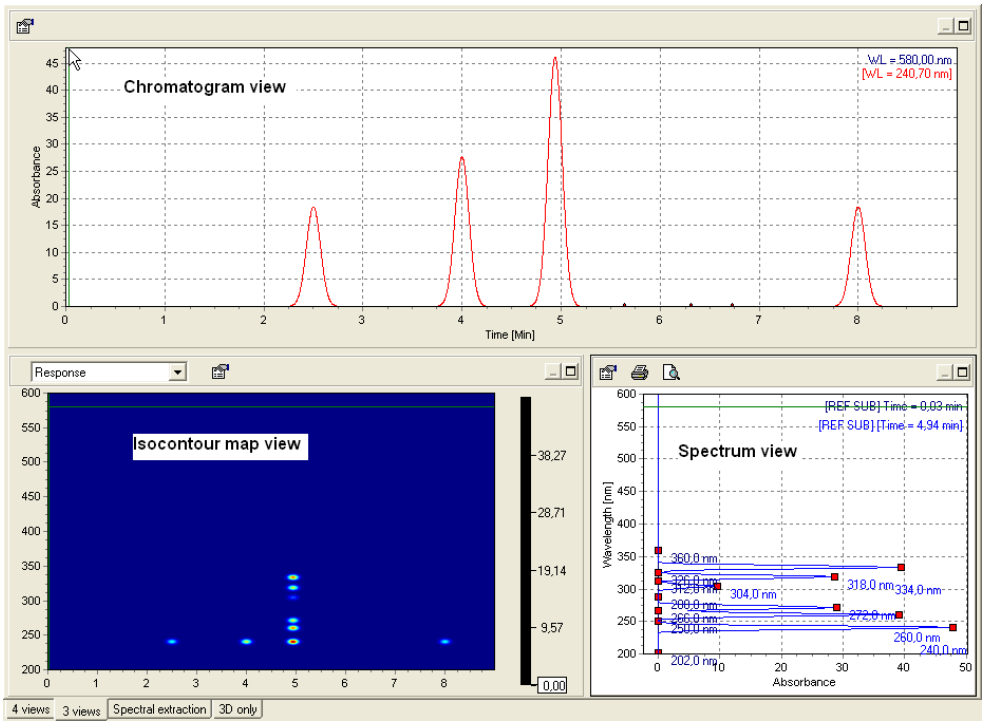


Choose the view(s) you want to display. All the views are linked : if one action is performed in one of the view (get chromatogram, get spectrum or normalization), it will automatically be applied in the other ones.

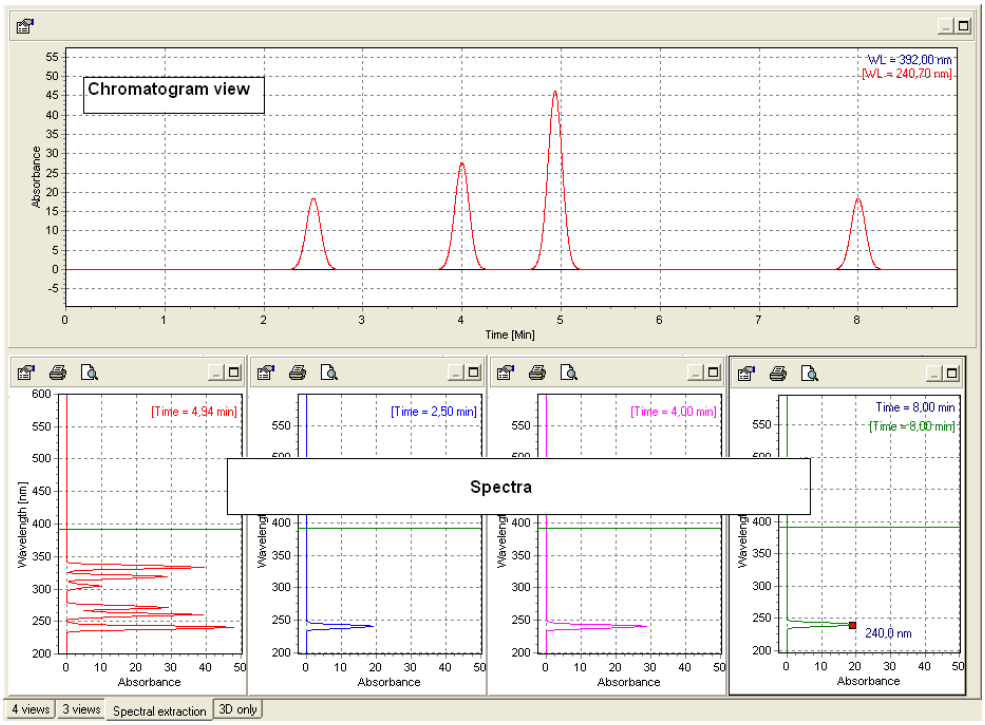
Each view is displayed in full page. Click on the corresponding tab to select the view to display.

The '3 views' consists of:

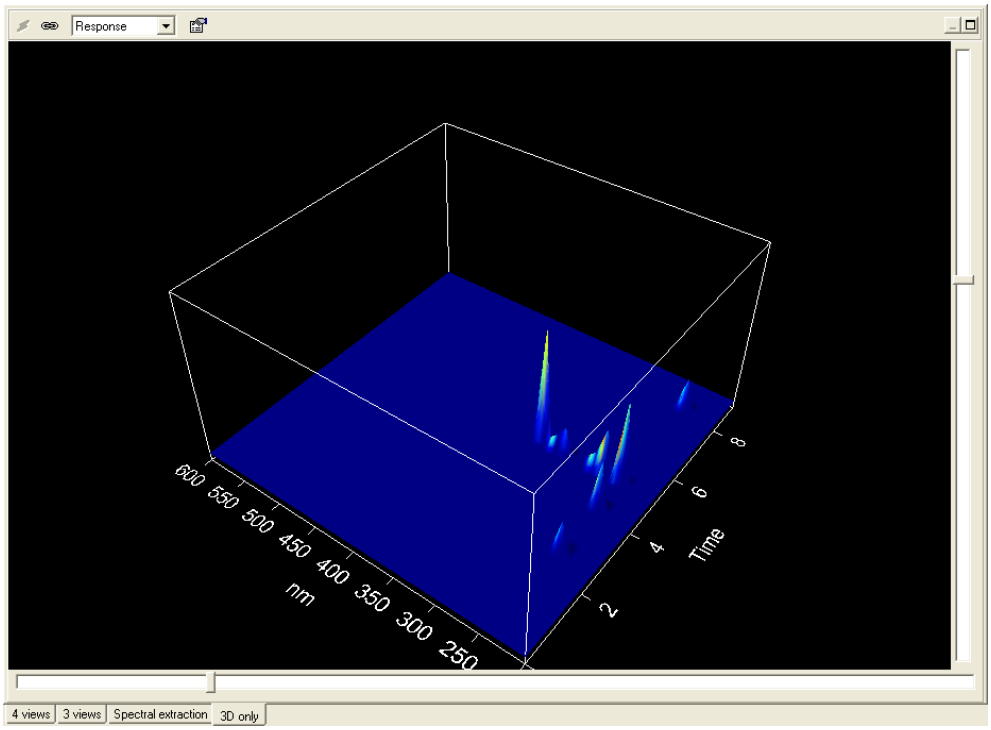
- The spectrum view.
- The chromatogram view.
- The isocontour view.



The 'spectral extraction' view contains one area with the chromatogram(s) and several area(s) (4 by default) with the spectra. The spectra field number can be changed using the spectra field pop-up menus. Select *Change spectra view number* and type the number of fields to be displayed.



The '3D only' view shows the data in a 3D view.



Modifying the display properties

The isocontour View

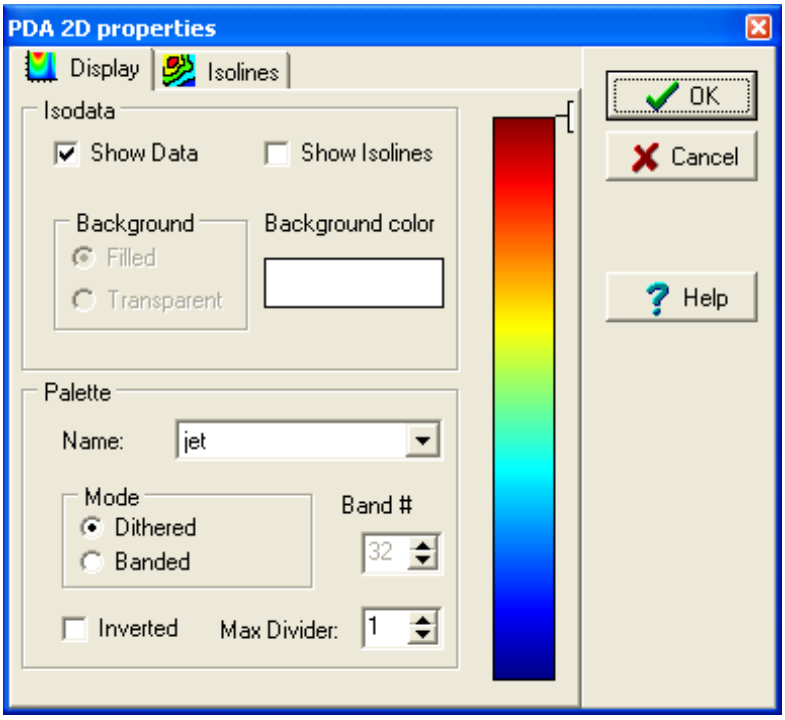
Use the following icons or scrolling list to:

	Modify the isocontour view properties, see below.
	Select which response you want to display. Four choices are proposed: Response, Threshold up, Threshold down and Threshold between to display respectively all the absorbance levels with the same importance or emphasize certain ones. All absorbances inferior to the lower limit or superior to the upper limit will have the same color.
	Maximize the isocontour map view to display it in the full area dedicated to PDA views
	Minimize the isocontour map view size and return in the preceding view mode.

Click on the button to change the isocontour view properties.

Two tabs allow you to modify the acquisition displaying properties: Display, Isolines.

Display



In this tab, customize the isocontour view display.

Check or uncheck **show data** to display or hide the acquisition points when *show isolines* is checked. If **show data** is unchecked, only the isolines are displayed.

Check or uncheck **show isolines** to display or hide the isolines.

If *show data* is unchecked, you can change the background color. Click on the mouse left button in the **background color** field and choose a color in the appearing screen. It is also possible to make the background transparent and display the scale grid (select **transparent** in the background field).

In the **palette** field customize the color scale of the view. The resulting scale is displayed on the screen right column. Change the **name** to modify the absorbance-color correspondence. It is also possible to invert the scale (check **inverted**) or to emphasize certain absorbances by changing the value of the **Max Divider** (see below for more explanation). The coloration can also be **dithered** or **banded**. In this case you can choose the number of bands.

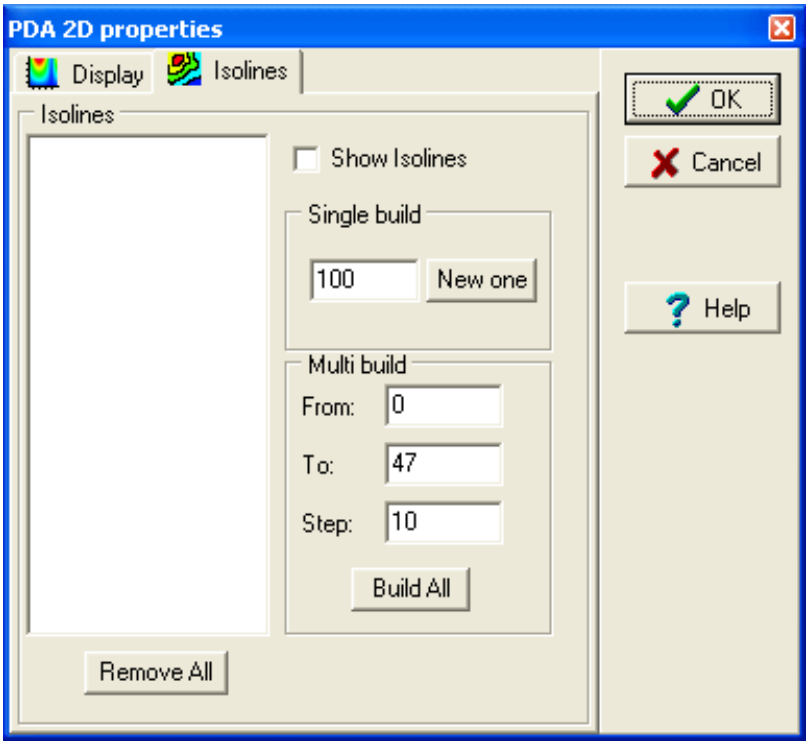
What does the Max Divider Parameter mean?

The Max Divider Parameter will define the limit of color levels displaying the isocontour view.

The inferior limit of the color level 7 (level for the largest absorbance values) will be divided by the max divider parameter. As a consequence, if Max Divider is superior to one, this level range will be larger and will contain more data points: above a certain value of absorbance, the data will be displayed with the same color (the color chosen for level 7).

The other color level ranges (1 to 6) will be narrowest. As a consequence, the small variations will be emphasized on the isocontour view.

In conclusion, if you want to emphasize the small variations of the isocontour display, choose a large value.



In the **Isoline** tab, check **Show Isolines** if you want to display isolines.

Choose the absorbance line you want to display in the single build field and then click on **New one**.

To automatically build the isolines, choose in the **Multi build** field, the minimum absorbance (From: field), the maximum absorbance (To: field) and the Step. Then click on *Build All.*

After choosing the isolines, their absorbance values are given in the Isolines field. You can uncheck the isolines you do not want to display.

The Chromatogram View

Colors of chromatograms are set by default and cannot be customized.

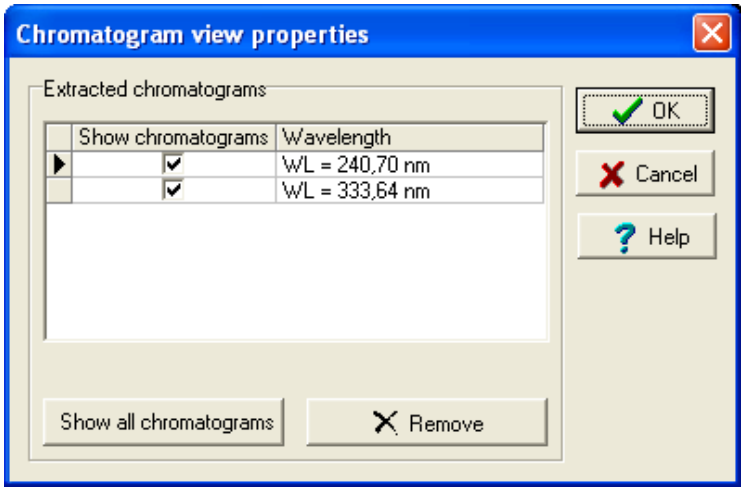
Use the following icons to:

Modify the chromatogram view properties, see below.

Maximize the chromatogram to display it in the full area dedicated to PDA views

Minimize the chromatogram view size and return in the preceding view mode.

Click on the button to change the chromatogram view properties. The following screen appears:



Choose which chromatogram(s) you want to display by checking the corresponding box in the *Show chromatograms* column.

Press the *Remove* button to delete chromatogram(s) you do not want to display.

Press the *Show all* button to display all the listed chromatograms.

The Spectrum View

Colors of spectra are set by default and cannot be customized.

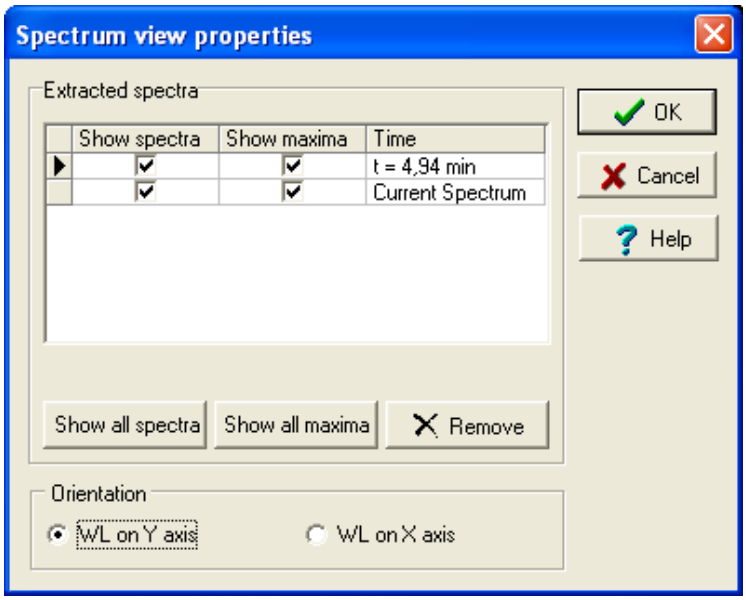
Use the following icons to:

Modify the spectrum view properties, see below.

Maximize the spectrum to display it in the full area dedicated to PDA views

Minimize the spectrum view size and return in the preceding view mode.

Click on the button to change the spectrum view properties. The following screen appears:



Choose which spectrum(a) you want to display by checking the corresponding box in the *Show spectra* column.

Choose which spectrum maximum(a) you want to display by checking the corresponding box in the *Show maxima* column. You can also choose to hide/show given maximum(a) by clicking on their box directly in the spectrum view.

Press the *Show all spectra* button to display all the listed spectra.

Press the *Show all maxima* button to display the maxima of all the selected spectra.

Press the *Remove* button to delete spectrum(a) you do not want to display.

Select the *WL on Y axis* or *WL on X axis option* to display the spectrum vertically or horizontally.

The 3D View

Use the following icons or scrolling list to:

Modify the 3D view properties, see below.

Response — Select which response you want to display. Four choices are proposed: Response, Threshold up, Threshold down and Threshold between to display respectively all the absorbance levels with the same importance or emphasize certain ones. All absorbances inferior to the lower limit or superior to the upper limit will have the same color.

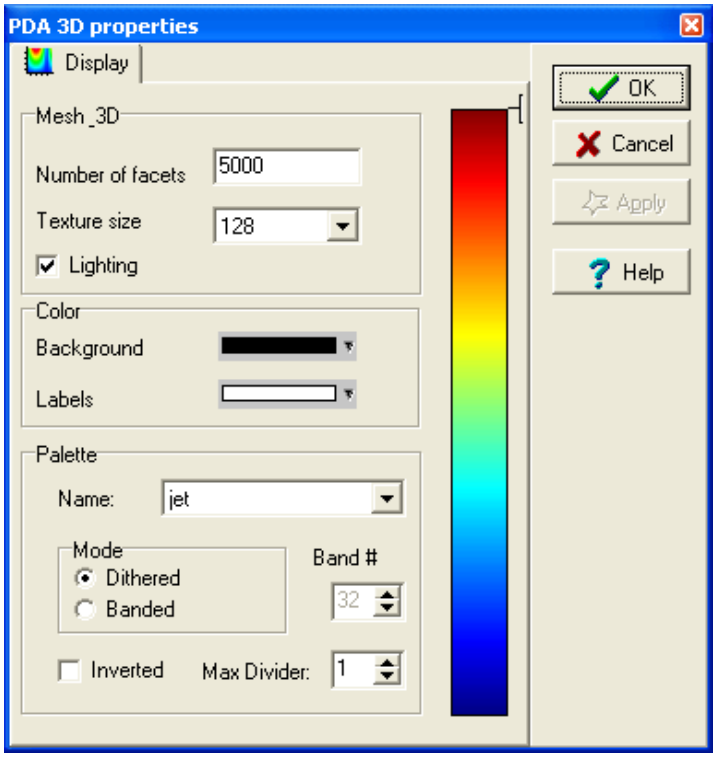
Create the 3D view. By default, the 3D view is empty.

Synchronize the zoom between the views.

Maximize the 3D view to display it in the full area dedicated to PDA views

Minimize the 3D view size and return in the preceding view mode.

Click on the button to change the 3D view properties. The following screen appears:



You can modify the appearance of the 3D object:

The number of facets and the texture size can be modified in the Mesh-3D field.

The color of the background and the labels can be chosen in the color field.

In the palette field customize the color scale of the view. The resulting scale is displayed on the screen right column. Change the name to modify the absorbance-color correspondence. It is also possible to invert the scale (check **inverted**) or to emphasize certain absorbances

by changing the value of the **Max Divider** (see below for more explanation). The coloration can also be dithered or banded. In this case you can choose the number of bands.

What does the Max Divider Parameter mean?

The Max Divider Parameter will define the limit of color levels displaying the 3D view.

The inferior limit of the color level 7 (level for the largest absorbance values) will be divided by the max divider parameter. As a consequence, if Max Divider is superior to one, this level range will be larger and will contain more data points: above a certain value of absorbance, the data will be displayed with the same color (the color chosen for level 7).

The other color level ranges (1 to 6) will be narrowest. As a consequence, the small variations will be emphasized on the 3D view.

In conclusion, if you want to emphasize the small variations of the 3D display, choose a large value.

Synchronization of the Views

In the '4views' or '3views' modes, you can apply the same zoom on all the views or work independently in each one. This can be done using the pop-up menus of each view.

Choose *Synchronized mode* to always synchronize the zoom in all the views.

Choose *Cursor mode* so that when you move the cursor in one of the views using the mouse, the corresponding chromatogram and/or spectrum is displayed in the corresponding view(s).

Unselect *Synchronized mode* in order to work independently in each views. It is nevertheless possible to synchronize punctually the chromatogram and/or spectrum afterwards with isocontour views using the following functions:

- *Synchronize views* from the isocontour popup menu: apply the same zoom on all the views.
- *Synchronize chromatogram with isocontour view* from the chromatogram popup menu: apply the isocontour view zoom on the chromatogram only. The spectrum(a) stay(s) unchanged.
- *Synchronize with isocontour view* from the spectrum popup menu: apply the isocontour view zoom on the spectrum only. The chromatogram(s) stay(s) unchanged.

Note: How to zoom: In each view, zoom in or out by clicking and dragging the left mouse button (from top-left to bottom-right to zoom in or bottom-right to top left to zoom out) or use the *Zoom in* or *Zoom Out* function of the pop-up menus.

Displaying Chromatograms and Spectra

Getting Chromatograms and Spectra

Many ways exist in CompassCDS Data System to fix chromatograms or spectra:

- First, you can fix the chromatogram or the spectrum at the current mouse cursor by clicking respectively on *get chromatogram* or *get spectrum* in each view pop-up menu.
- You can also fix a chromatogram or a spectrum by keyboard typing the wavelength value or the time. Click on *Get chromatogram at WL* in the chromatogram popup menu or *Get spectrum at time* in the spectrum popup menus of each view.
- At least, you can fix spectra by enabling the *Spectrum selection* function in the chromatogram popup menu of the 'spectral extraction' mode. Select the area where you want to display the spectrum(a). Now, move the cursor over the chromatogram and double click once the cursor is correctly positioned to fix the spectrum. Several spectra can be fixed successively still *Spectrum selection* is enabled.

Once chromatograms and spectra have been fixed you can display or hide them in each view. Press the button and in the appearing screen respectively check or uncheck the chromatogram(s) or spectrum(a). Press the *remove* button to delete chromatogram(s) or spectrum(a) you do not want to display. Press the *display all* button to display all the chromatogram or spectra listed above.

The maximum absorbance chromatogram can also be displayed. Choose *Show max absorbance chromatogram* in the chromatogram pop-up menus of the '4views', '3views' or 'spectral extraction' views. The maximum absorbance wavelength is given at each chromatogram points when you move the mouse cursor over the chromatogram.

Note: The maximum absorbance chromatogram is a virtual chromatogram which shows all components at their maximum absorbance. Within the selected wavelength range (full range or user defined range), CompassCDS takes the highest absorbance value from the spectrum and uses it as a chromatogram data point to generate the 2D chromatogram data field (spectrum time as x-value, highest absorbance value as y value). This chromatogram is very useful for quantitative calculation. The wavelength at which the maximum absorbance has been found is displayed in the top of the chromatogram when you left click on the chromatogram.

Normalization of the Spectra Views

Use the normalization function to apply a specific scale on the spectra absorbance axis. This can be done from the spectrum popup menus of the '4views', '3views' or 'spectral extraction' views.

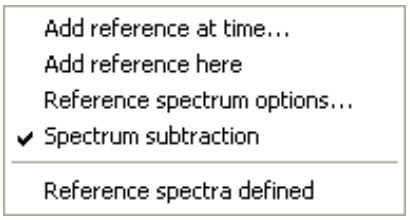
Click on *Normalized View,* a submenu is displayed with two choices (**auto** and **at WL**). Depending on the chosen option, the spectra are zoomed in such a way that the signal corresponding to the maximum absorbance (auto mode) or the absorbance at the specified wavelength of all the displayed spectra (**at WL** mode) represents 5 to 95% of the absorbance axis.

Spectrum Subtraction

Use the Spectrum subtraction function to subtract one spectrum (got at a specific time) or the spectrum interpolated between two reference spectra to all other spectra. This can be

done from the chromatogram popup menus of the '4views', '3views' or 'spectral extraction' views.

Click on the *Spectrum subtraction* option to select a spectrum to subtract. The following screen appears:



Choose **Add reference at Time** and enter manually a time where a reference spectrum will be defined in the appearing screen.

Click on **Add reference here** to define a reference spectrum at the cursor time.

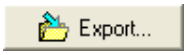
Choose **reference spectrum options** to remove some reference spectra.

Check **Spectrum subtraction** to activate or not the subtraction. A spectrum is interpolated between two consecutive reference spectra and subtracted to all spectra of the corresponding interval. The results of the subtraction are given in the spectrum view.

When reference spectra have been defined, "Reference spectra defined" appears in the bottom part of that popup menu. Else, "No reference spectrum defined" appears.

The ASCII Export of Spectra

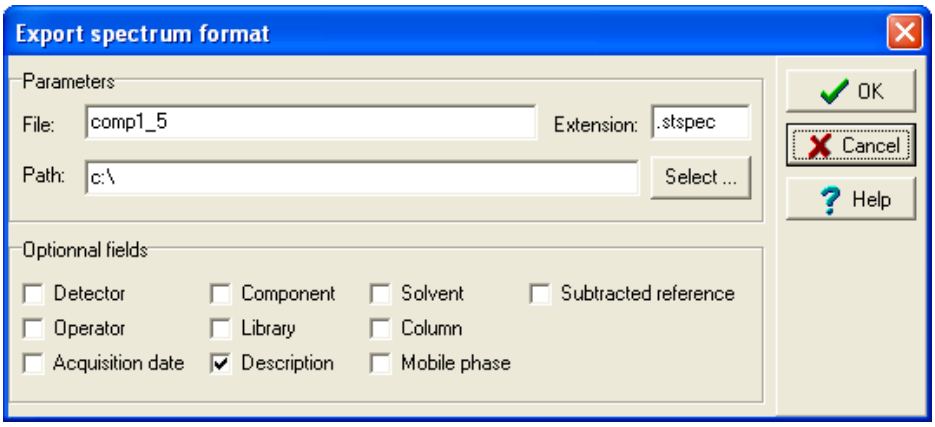
Spectral Data can be exported with the ASCII format.

To perform this export, click on the 

button in the Spectral Library Editor window to export a spectrum stored in a library.

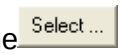
Otherwise, from the spectrum view of the 3-view, 4-view or spectral extraction mode, use the pop-up menu and the 'Spectrum processing' then 'Export spectrum' option.

The following screen appears:



This window is divided into 2 parts, the 'Parameters' of the export and some 'Optional Fields' if a reference spectrum from a library is to be exported and 3 parts if a spectrum from a spectrum view is going to be exported.

In the 'PARAMETERS' part, you can choose the name of the spectrum listed in the library you want to export and the path where you want to export this file. Be sure you have writing rights on the export directory.

You can type in the export path or use the 

button to use a browser to select it.

In the 'OPTIONAL FIELDS', you can check boxes corresponding to the information you want to export:

- Detector: if this box is not checked, the name of the detector the spectrum was recorded with, will not be exported.
- Operator: if this box is not checked, the name of the operator who ran the acquisition of the spectrum will not be exported.
- Acquisition date: if this box is not checked, the acquisition date of the spectrum will not be exported
- Component: if this box is not checked, the component information corresponding to the spectrum will not be exported
- Library: if this box is not checked, the name of the library the spectrum was stored in will not be exported.
- Description: if this box is not checked, the description of the not be exported
- Solvent: if this box is not checked, the solvent information (if any) will not be exported
- Column: if this box is not checked, the column information (if any) will not be exported
- Mobile Phase: if this box is not checked, the mobile phase information (if any) will not be exported
- Subtracted reference: if this box is not checked, the name of the reference spectrum subtracted to the exported spectrum will not be exported.

Once the export parameters have been set, click on the *OK* button. The following message appears then, informing the user that the export is successful:

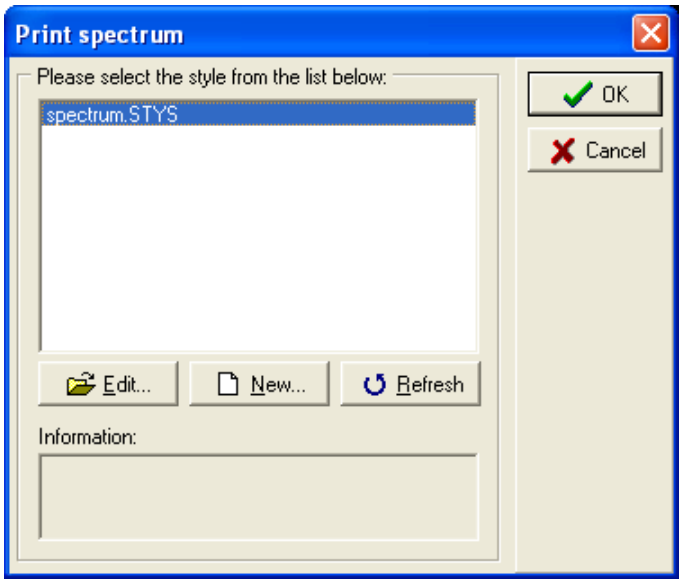
Note: See page 44 for more details about the CompassCDS ASCII format.

The Spectra Report Editor

CompassCDS Spectra Report Editor enables you to generate, customize, and print spectral reports from the CompassCDS.

This feature is accessible from the spectra view (in the 4-view, 3-view and spectral extraction modes), it is possible to preview or print a spectra report by clicking either on the or the buttons.

The following screen is displayed:



When the user selects a defined report in the list, he can edit it by pressing the *Edit* button; create a new one by pressing the *New* button to customize the report, or refresh the list by pressing the *Refresh* button.

The CompassCDS Spectrum Report editor is open where user can choose to add standard objects and Spectra Report Object.

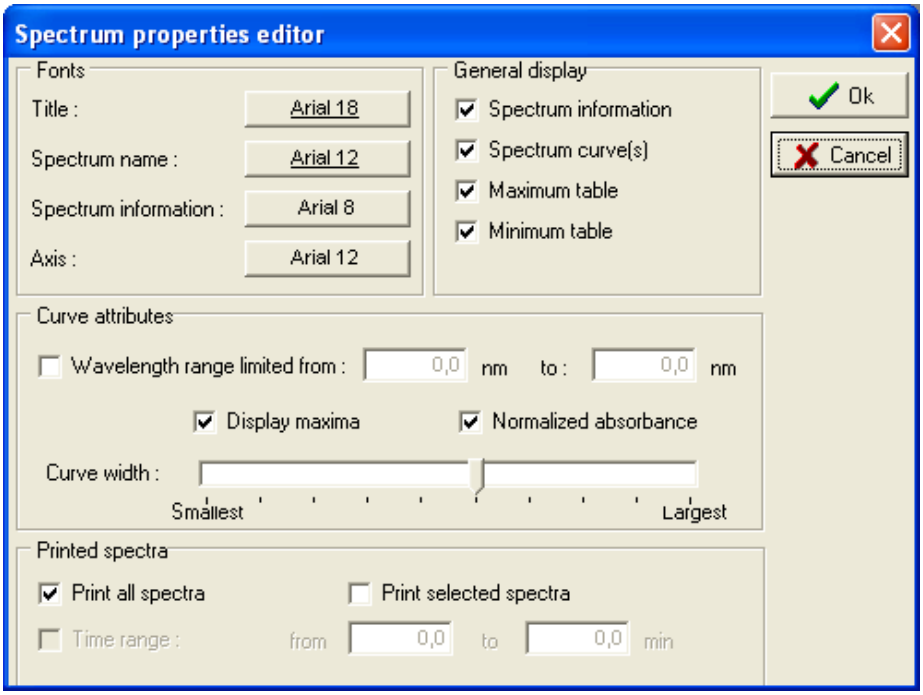
Standard Objects

Concerning standard object such as text, table or graphic objects, please refer to the CompassCDS report Editor Manual.

Spectra Report Object

This object enables you to create and to insert a spectra report. You can define the spectra to print, font style, and general display parameters.

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



In the '*Fonts*' part, you can choose the font of the different items that are to be printed such as the title or the spectra names police size.

In the *General Display* part, you can check the boxes corresponding to:

- Library header: if this box is not checked, the name of the printed library, the number of reference spectra listed, the creation date and description will not be displayed on the report.
- Spectrum table: if this box is not checked, information on the spectra present in the library (such as the compound names, the retention times, and their description and acquisition window) will not be printed.
- Spectrum information: if this box is not checked, information on the printed spectra (such as the name of the chromatogram file it was extracted from, the detector name of the system, the experimental conditions (solvent, column) or the acquisition date) will not be printed in the report.
- Spectrum curve: if this box is not checked, no spectrum curve will be printed in the report
- Maximum table: if this box is unchecked, the wavelength at the maximal absorbance and the value of the maximal absorbance will not be displayed on the report.
- Minimum table: if this box is unchecked, the wavelength at the minimal absorbance and the value of the minimal absorbance will not be displayed on the report.

In the *'Curve Attribute'* part, you can customize the curve by setting the wavelength range that will be printed, if maxima will be displayed, if the absorbance will be normalized or not and the width of the drawing

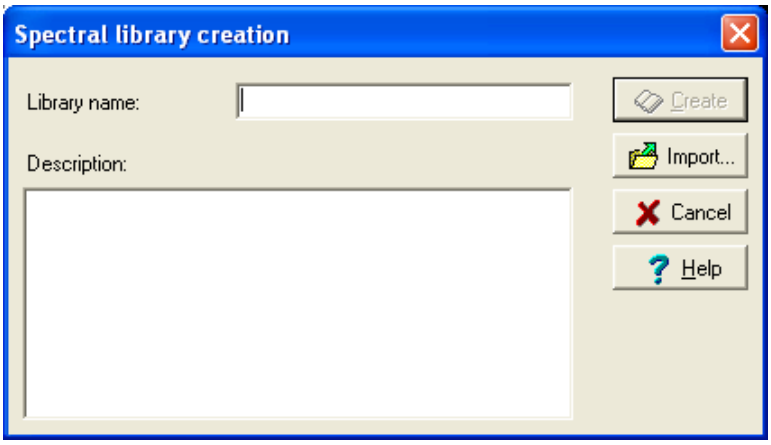
Finally, you can choose which spectra are to be printed: all of them, any consecutive ones listed in the library, those corresponding to a defined time range, or only the ones named in this screen.

PDA Data Processing

The Spectral Library Editor

Creating a New Library

In the **File** menu, click on the *New / New spectral library* option. The following screen appears:

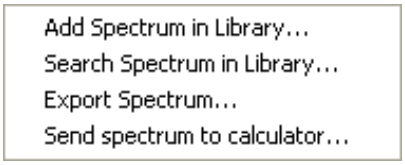


Enter the name of the new library and then click on the *Create* button. User can also add a description. This description will then be displayed when selecting this library in the other screens.

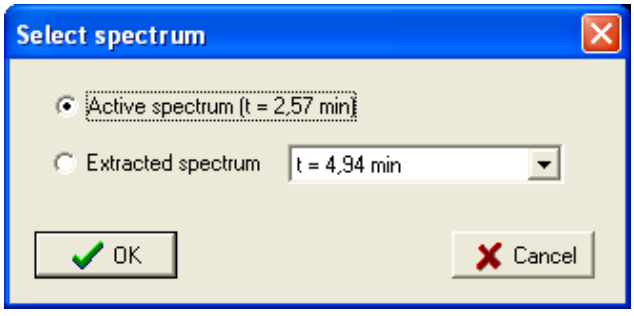
Click on the *Import* button to import in one step several ASCII spectra in a Library. You can give it a name or recover the name of an old library (exported from the Star Software).

How to Fill the Spectral Library

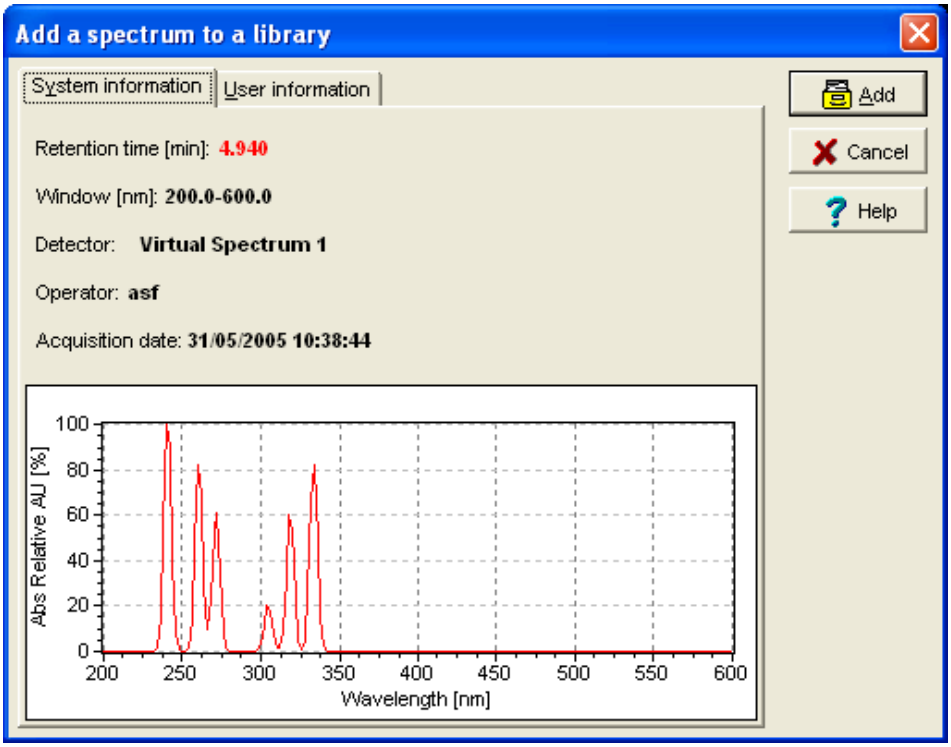
You can add specific spectrum in the library using the pop-up menus of different areas: the spectrum field (from the '4 views' '3 views' or 'spectral extraction' screens) or the isocontour field (from the '4views' or '3 views' screens). Right-click and choose the **Spectrum processing** menu and the following sub menu appears:



Now choose **Add Spectrum to Library** and select which spectrum you want to add in the following sub menu:



The following screen appears:

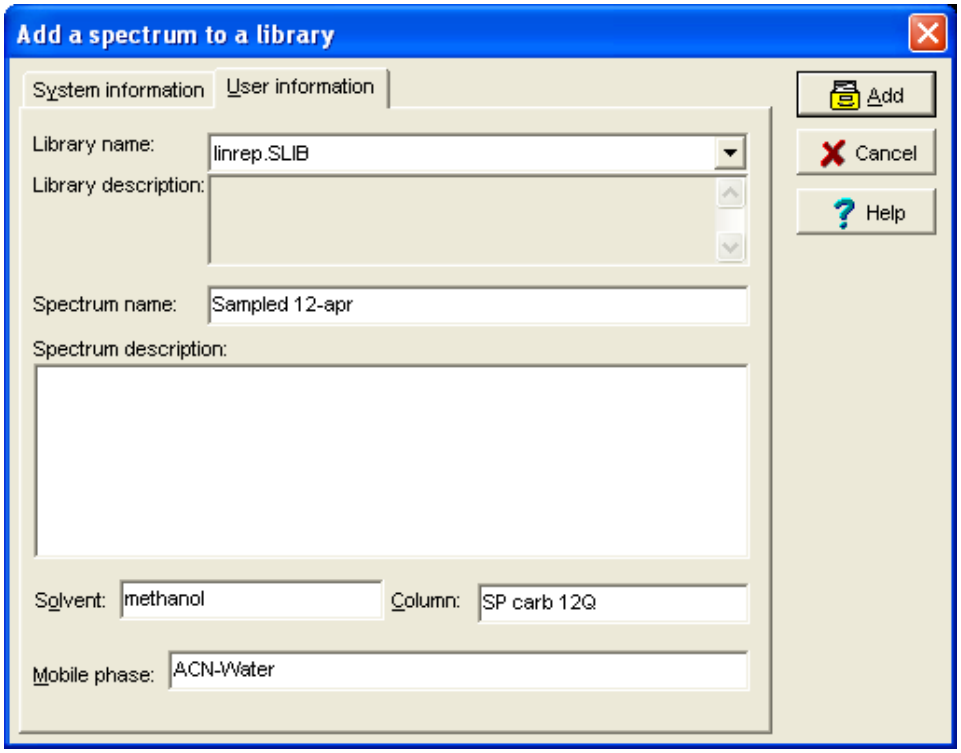


The following is displayed on this page:

- The retention time from which the spectrum is extracted.
- The acquisition wavelength range (Window field)
- The detector type
- The operator name
- The acquisition date

The added spectrum is displayed in this page. Click on the *Add* button to add the selected spectrum. Click on *Cancel* to close the library without adding the selected spectrum.

Click on the ***User Information*** tab. The following screen appears:

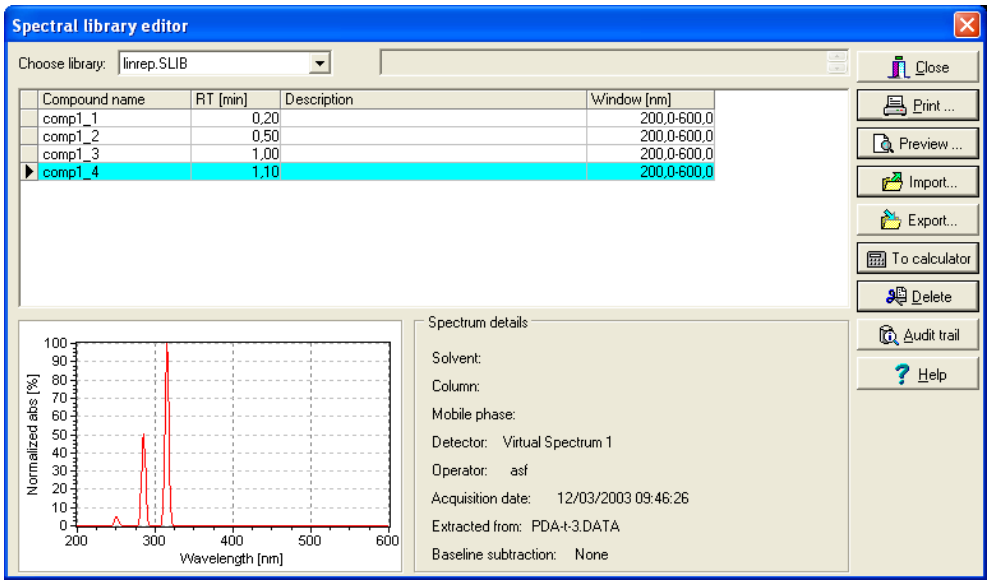


In the **Library name** field, choose a library using the scrolling list. The description entered at library creation is automatically displayed in the Library description field.

Enter the spectrum name and optionally, any description concerning the extracted spectrum. Additional information can be entered such as **Solvent** name, **Column** type, **Mobile Phase.**

Open a Library

In the **File** menu, click on *Open / Open spectral library*. The following screen appears:



In the **Choose library** field, choose a library using the scrolling list. If spectra are stored in this library:

- the name of the spectrum appears in the compound name
- the acquisition wavelength range is specified in the Window column

When you choose one spectrum, the spectrum curve appears in the left part of the screen and the different fields (Solvent, Column, Mobile Phase, Detector, Operator, Acquisition date, Extracted from and baseline subtraction) are filled. This information is given by the user when a spectrum is added to the library, see page 41.

To delete a spectrum, click on its name and then on the *Delete* button.

The ASCII Import of Spectra

Spectra can be imported with the ASCII format.

From the Spectral Library, click on the

button.

An 'Open' box opens and the user is asked to select in the Windows browser the file he wants to import.

The newly imported spectrum is then displayed with all the information contained in it: experimental conditions, operator, acquisition date, etc.

In the description field, 'imported' is displayed to warn the user this spectrum has been imported

The CompassCDS ASCII format of spectra

Mandatory Data

Chromato Extracted From:	Name of the chromato file, the spectrum had been extracted.
RT:	Time of the extracted spectrum.
Number of Points:	Number of points in the spectrum
x0 : y0 :	Points List: x ⇔ Time, y ⇔ Absorbance.
.	
.	
xn : yn :	

Additional Data

Component Name:	Name of the component spectrum.
Library Name:	Name of the library the spectrum comes from.
Acquisition Date:	Date of the chromato acquisition / spectrum extraction (“MM/DD/YY HH:MM:SS”)
Description:	Spectrum description.

Detector:	Name of the detector used for acquiring this spectrum
Operator:	Name of the operator who performed this spectrum acquisition
Solvent:	Name of the solvent used for acquiring this spectrum
Column:	Name of the column used for acquiring this spectrum
Mobile Phase:	Name of the mobile phase used for acquiring this spectrum.
Ref Subtracted; RST:	Has a reference spectrum be subtracted to the extracted one? And Time of the reference spectrum if any.

Other Conventions

Fields Separator:	**;**
Decimal separator:	**.**
File extension:	

Suggestions:

Another ASCII file could be defined to describe the library grouping different spectra, with fields like:

- Library Name
- Library Description
- Library History

The Spectral Library Report Editor

CompassCDS Spectral Report Editor enables you to generate, customize, and print spectral reports from the CompassCDS.

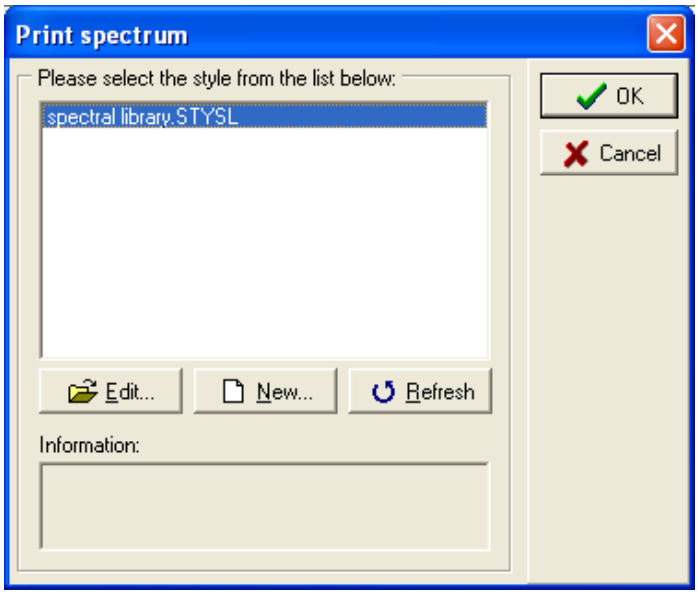
In CompassCDS Report Editor, all the objects can be placed and sized inside pages as they will be printed.

The CompassCDS Report Editor graphical environment is composed of a main menu, toolbars, a browser, a working space, and a status bar.

To print or print preview a Spectral Library, open it then click on the

or

icon. The following screen is displayed:



When the user selects a defined report in the list, he can edit it by pressing the *Edit* button, create a new one by pressing the *New* button to customize the report, or refresh the list by pressing the *Refresh* button.

The CompassCDS Spectrum Report editor is open where user can choose to add standard objects and Spectra Report Object.

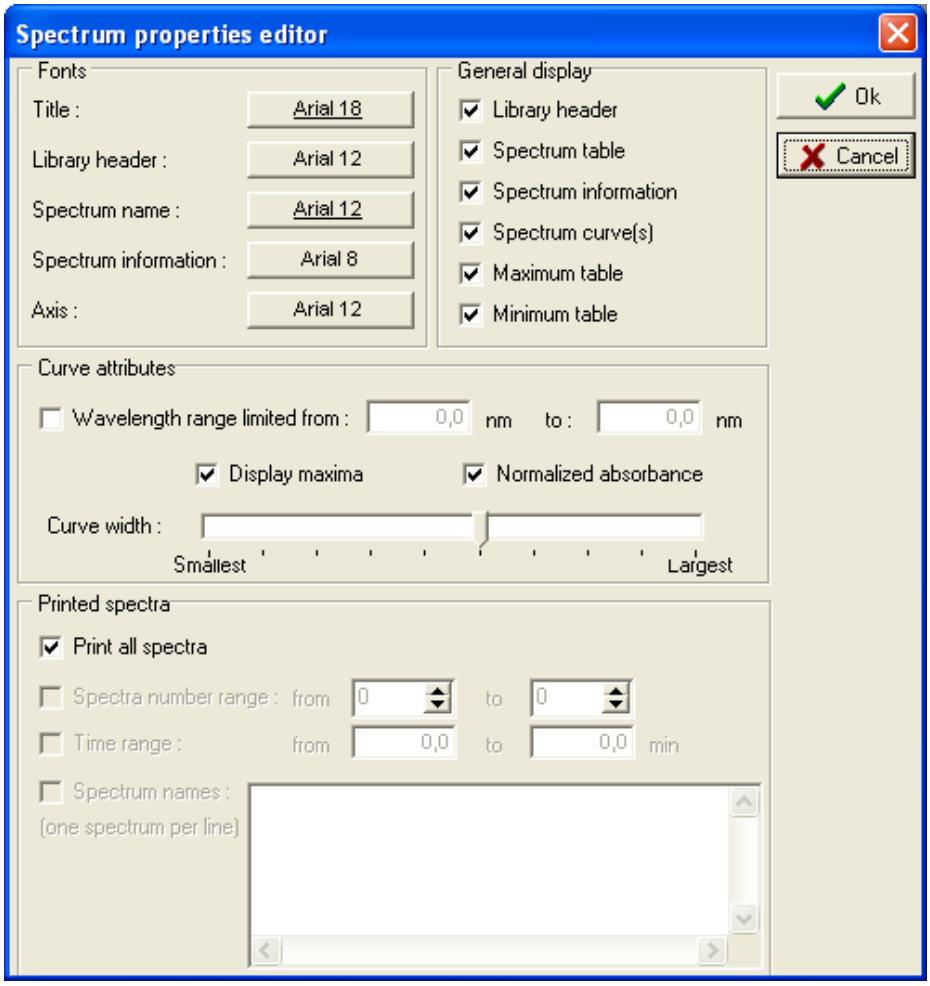
Standard Objects

Concerning standard object such as text, table or graphic objects, please refer to the CompassCDS report Editor Manual.

Spectra Report Object

This object enables you to create and to insert a spectra report. You can define the spectra to print, font style, and general display parameters.

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



In the '*Fonts*' part, you can choose the font of the different items that are to be printed such as the title or the spectra names police size.

In the *General Display* part, you can check the boxes corresponding to:

- Library header: if this box is not checked, the name of the printed library, the number of reference spectra listed, the creation date and description will not be displayed on the report.
- Spectrum table: if this box is not checked, information on the spectra present in the library (such as the compound names, the retention times, the description and acquisition window) will not be printed.
- Spectrum information: if this box is not checked, information on the printed spectra (such as the name of the chromatogram file it was extracted from, the detector name of the system, the experimental conditions (solvent, column) or the acquisition date) will not be printed in the report.
- Spectrum curve: if this box is not checked, no spectrum curve will be printed in the report
- Maximum table: if this box is unchecked, the wavelength at the maximal absorbance and the value of the maximal absorbance will not be displayed on the report.

- Minimum table: if this box is unchecked, the wavelength at the minimal absorbance and the value of the minimal absorbance will not be displayed on the report.

In the *'Curve Attribute'* part, you can customize the curve by setting the wavelength range that will be printed, if maxima will be displayed, if the absorbance will be normalized or not and the width of the drawing

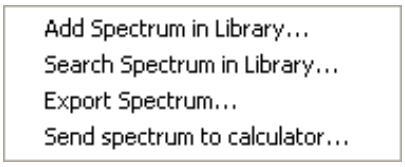
You can finally choose which spectra are to be printed: all of them, any consecutive ones listed in the library, those corresponding to a defined time range, or only the ones named in this screen.

The Library Search

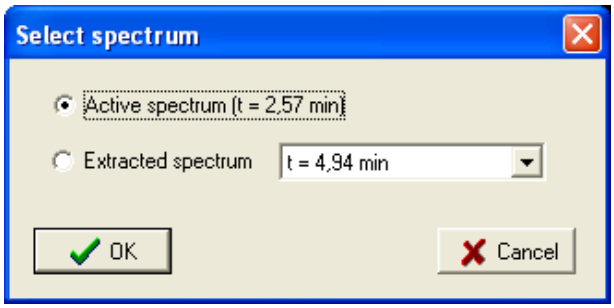
This option allows the operators to identify an unknown spectrum by searching the similar spectrum in the library. This option can be used manually or automatically. The manual search is useful to define the appropriate search parameters or to quickly identify some unknown. The manual search can also find the library spectrum to be used as reference for purity calculation. A link exists which allows to define this reference spectrum directly from the manual search screen.

The Manual Search

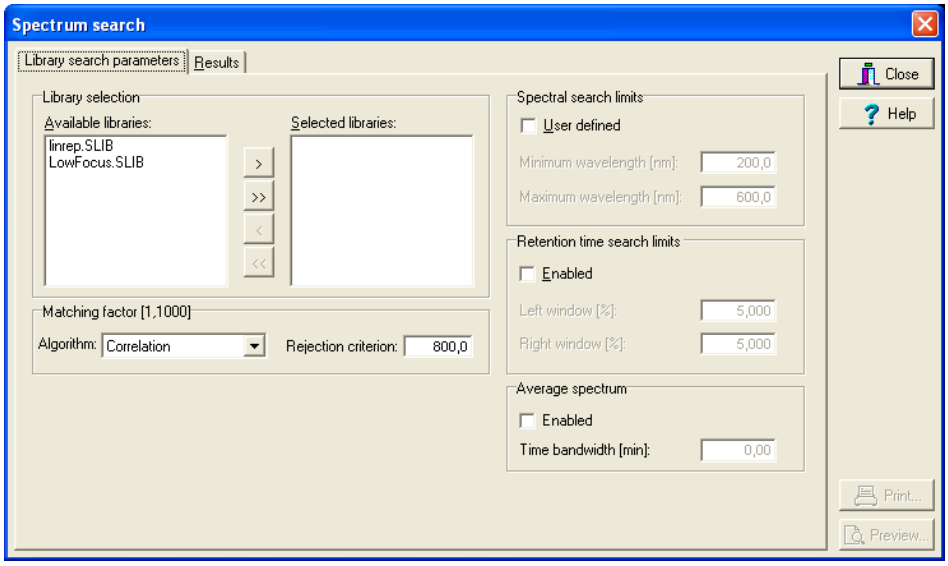
The manual search can be performed using the pop-up menus of different views: spectrum pop-up menus (from the '4 views', '3 views' or 'spectral extraction' views) or isocontour pop-up menu (from the '4views' or '3 views' views). Right-click and choose the **Spectrum processing** menu and the following sub menu appears:



Now choose **Search spectrum in Library** and select which spectrum you want to compare in the following screen:

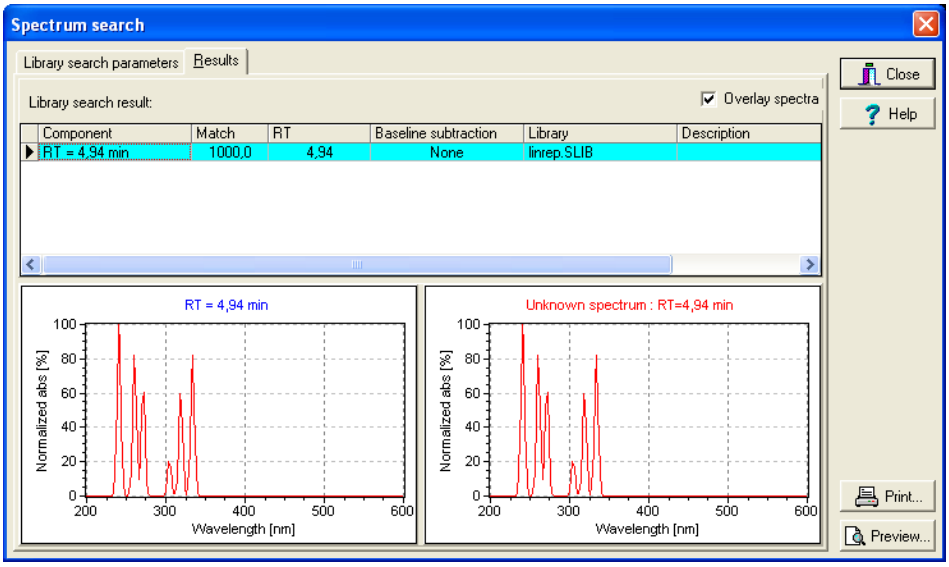


The Spectrum Search screen consists of two tabs. Choose the **Parameters** one. The following screen appears:



Select the parameters used to search the spectrum in the libraries. The parameters definition is given beginning on page 52.

Click on the *Results* tab, the following screen appears:



The correlations are calculated and the candidate spectra are displayed in the spectrum table. For an unknown spectrum, the table gives the library spectrum name, its retention time, the matching factor, the library it comes from and the baseline subtracted if any. The components are listed in their matching factor order.

Select a table line to display the corresponding component curve in the field at the bottom of the window. By default, the **overlay spectra** box is unchecked and the spectra are displayed on different windows. The unknown and library spectra can be overlaid. (Check the **overlay spectra** box.)

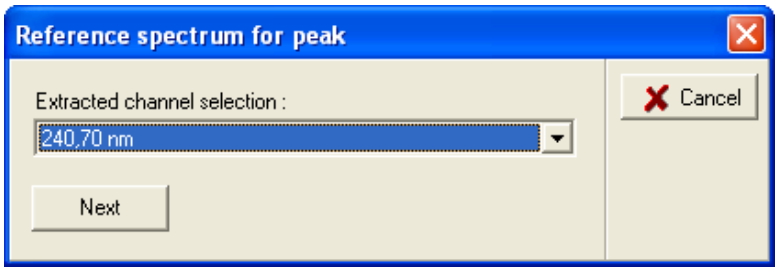
In both cases, the spectra are normalized to 100%.

Note: The results of a manual search cannot be saved

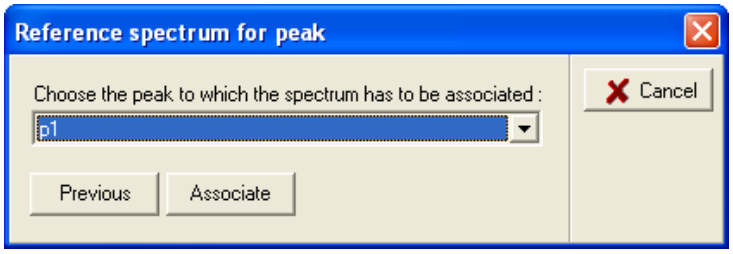
Use the or button to print or print preview the results (see the Manual Library Search Editor section page 50 for details).

Link with the Peak Identification Table of Peak Purity Calculations

It is also possible, from the result tab, to define which library spectrum must be used as reference for purity calculations. Right -click on the spectrum you want to use as reference and click on *Reference spectrum for purity computations.* The following screens appear:



In this screen, select the extracted chromatogram in which the reference spectrum will be associated. Press *next* to display the following screen:



Now, choose the peak to which the spectrum must be associated and press *associate* to associate them.

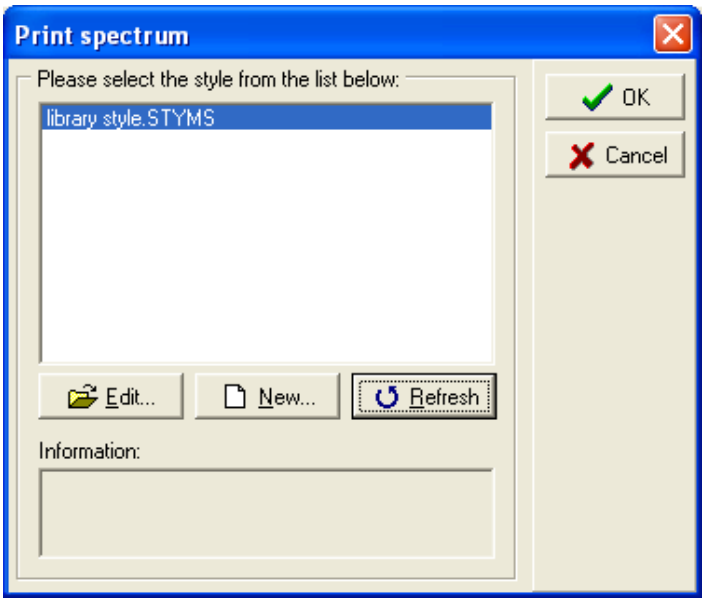
The Manual Library Search Report Editor

CompassCDS Library Search Report Editor enables you to generate, customize, and print manual library search results reports from the CompassCDS.

In CompassCDS Report Editor, all the objects can be placed and sized inside pages as they will be printed.

The CompassCDS Report Editor graphical environment is composed of a main menu, toolbars, a browser, a working space, and a status bar.

To print or pint preview Manual Library Search results, click on the Print ... or Preview ... button. The following screen is displayed:



When the user selects a defined report in the list, he can edit it by pressing the *Edit* button; create a new one by pressing the *New* button to customize the report, or refresh the list by pressing the *Refresh* button.

The CompassCDS Manual Library Search report editor is open where user can choose to add standard objects and Library Search Report Object. Please refer to the CompassCDS report Editor Manual for details.

The Automatic Search

The parameters of the automatic library search are defined in the spectrum method part and are the same for all extracted chromatograms. In the method sub-section of the spectrum section, click on the Edit library search... button to display the screen which allows the user to configure the library parameters (The parameters definition is given beginning on page 43.).

The results for the best matching component can be displayed in the peak results table. Add the Matching component, the matching factor and the matching component library variables (right-click on the peak result table and then choose *report properties*) in the report. Three additional columns appear:

#	Name	Time [Min]	Quantity [% Area]	Area [µV.Min]	Matching Comp	Match.Factor	Matching Comp
1	UNLNOWN	2,48	11,75	17610,5	Benzene	999,794	Demo.SLIB
2	UNKNOWN	4,02	15,78	23641,8	Anthracene	999,996	PAH.SLIB
3	UNKNOWN	5,01	51,59	77304,4	Pyrene	999,955	PAH.SLIB
4	UNKNOWN	7,93	20,89	31297,1	Perylene	999,999	PAH.SLIB
Total			100,00	149853,8			

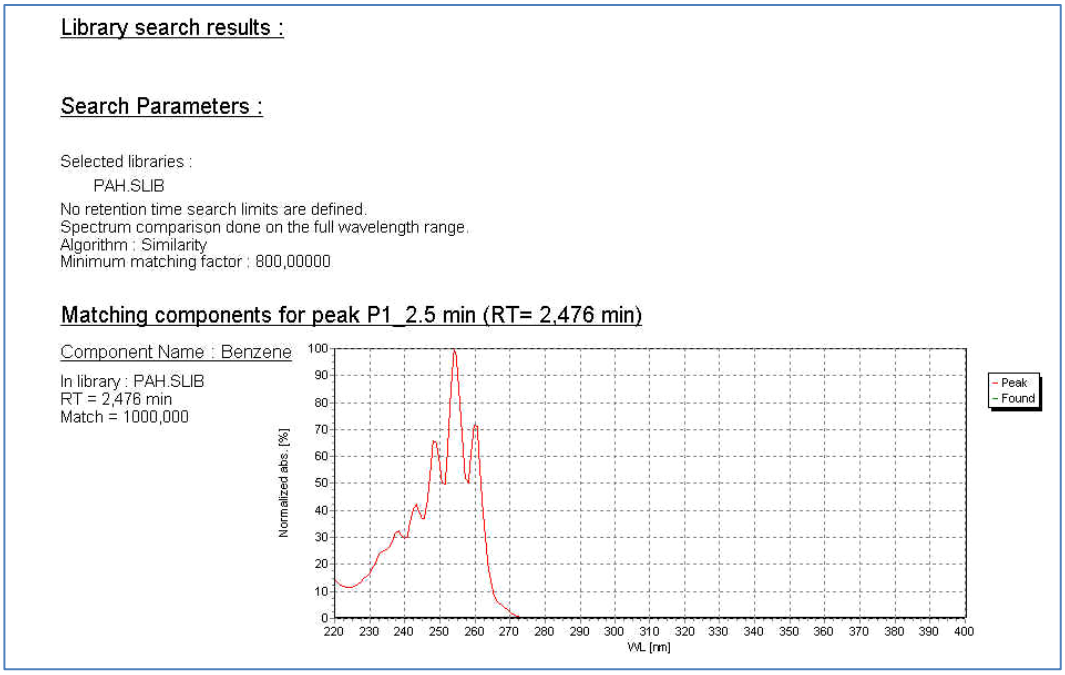
This table can be printed using the peak table object of the CompassCDS Report Editor. Refer to the CompassCDS Report Editor User Guide to see how to build the report style.

The whole library search results can also be displayed or printed via the report editor (CompassCDS Report Editor).

First, define a report style in CompassCDS Report Editor. This style must include a library search object. Refer to the CompassCDS Report Editor User Guide to see how to build the report style.

Then, choose this style in the report sub part of the extracted chromatogram method and click on the button to display a preview of the report or the button to print it.

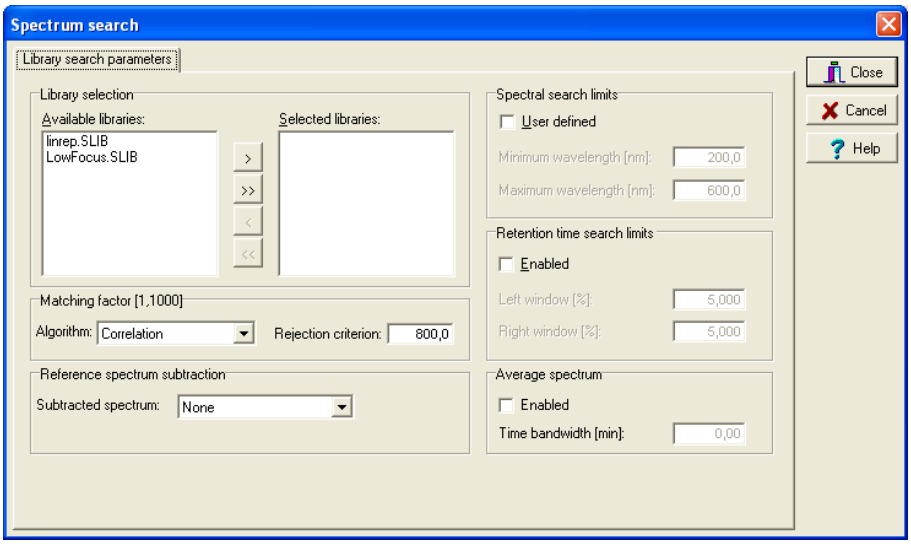
For example, the following image shows a report including the library search results.



According to the CompassCDS Report Editor object properties, the libraries and parameters used for the search can be printed and for an unknown spectrum, the report gives the library spectrum name, its retention time, the matching factor and the library from which it is extracted.

The Search Parameters

Several parameters must be defined to search a spectrum in the library.



Library selection: The unknown spectra can be compared to spectra of several libraries (all spectra of the libraries listed in the *selected libraries* field). To select the libraries choose one or more libraries in the *Available libraries* list and click on the > button to move them in the *Selected libraries* list. Click on >> to select all the available libraries. Click on the < or << button to remove one or all the libraries listed in the *selected libraries* list.

Spectral search limits: By default, the search is realized on the entire spectral range of the unknown (*User defined* box is unchecked) but the user can limited the search in a spectral window (check the *User defined* box and type the chosen value in the appropriate field now enabled). The unknown spectrum will be compared only to library spectra which wavelength ranges are equal or greater than the unknown spectra.

For example:

Unknown spectra **|----------|**

Library spectrum 1 |----------|

Library spectrum 2 |----------|

Library spectrum 3 |----------|

The unknown spectrum will be compared to spectrums 1 and 2, but not to spectrum 3.

Retention time search limits: by default, all library spectra are taken into account for calculation (the *Enabled* box is unchecked). But the user can defined a smaller time window. The unknown spectrum will be compared to spectra which time corresponds to the following formula:

$T_r-\Delta T_g \leq T_{ri} \leq T_r+\Delta T_d$

where T_r is the unknown spectrum retention time

ΔT_g and ΔT_d are the left and right time window

T_{ri} is the library spectrum retention time.

Matching factor: choose the algorithm to use and the Rejection Criterion value, which is the matching factor limit value under which a spectrum from the library is not considered to identify the studied spectrum. Three matching algorithms exist in CompassCDS.

Reference spectrum subtraction: (available in automatic mode only): choose the spectrum to be subtracted. You can select a spectrum to correct the background absorption (this background absorption can be different if the solvent is different from one analysis to another).

- Choose **None** to subtract no spectrum
- Choose **Manual reference** to manually define the time where the spectrum must be extracted. An additional box is added behind the scrolling list where the time can be entered.
- Choose **Peak baseline average** to subtract the spectrum interpolated between peak start and peak stop markers.

Average spectrum: (available in automatic mode only): check *enabled* and define the *time bandwidth* in the enabled field. In that case the spectra compared with the library will be the average of spectra obtained at peak apex over the defined time bandwidth.

The Library Search Results Print

The library search results can be printed as a whole using the report editor (CompassCDS Report Editor).

First, define a report style in the CompassCDS Report Editor. This style must include a library search object. Refer to the CompassCDS Report Editor User Guide to see how to build the report style.

Then, choose this style in the report sub part of the extracted chromatogram method and select 1 in the copy number field. Click on the *preview* button to display the report.

According to the CompassCDS Report Editor object properties, the libraries and parameters used for the search can be printed and for an unknown spectrum, the report gives the library spectrum name, its retention time, the matching factor and the library from which it is extracted.

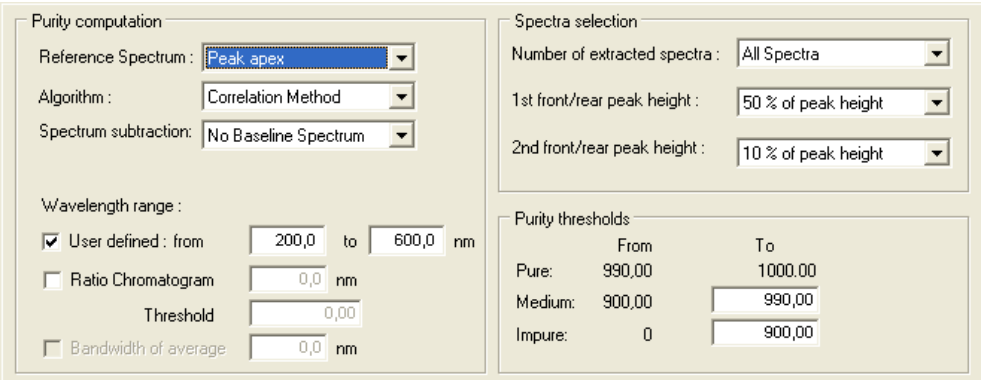
These results can be printed automatically after the acquisition (if the correct report style is defined in the report part of the acquisition method) or manually using the button.

The name of the component that better matches the unknown spectra, the corresponding matching factor and the library it comes from can also be printed. Add in the report a peak table object and associate it a format containing the three variables MATCHCOMPONENT, MATCHFACTOR and MATCHLIBRARY.

The Peak Purity

The Peak Purity Calculation

The peak purity calculation informs the user if a peak is composed of one or several components. In case of co-eluting components, the purity will be very low. The purity test is based on the comparison of spectra stored during the peak elution. Click on the peak purity part of the extracted chromatogram method. The following screen appears:


Purity computation
Reference Spectrum : Peak apex
Algorithm : Correlation Method
Spectrum subtraction: No Baseline Spectrum
Wavelength range :
User defined : from 200,0 to 600,0 nm
Ratio Chromatogram 0,0 nm
Threshold 0,00
Bandwidth of average 0,0 nm
Spectra selection
Number of extracted spectra : All Spectra
1st front/rear peak height : 50 % of peak height
2nd front/rear peak height : 10 % of peak height
Purity thresholds
From To
Pure: 990,00 1000.00
Medium: 900,00 990,00
Impure: 0 900,00

In the **spectra selection field**, you have to choose:
***the number of extracted spectra*.**

Generally, 3 spectra by peak are used to calculate the purity. If necessary, choose apex only, 7 or all spectra.

Now, choose ***the location of these spectra*** in the peak

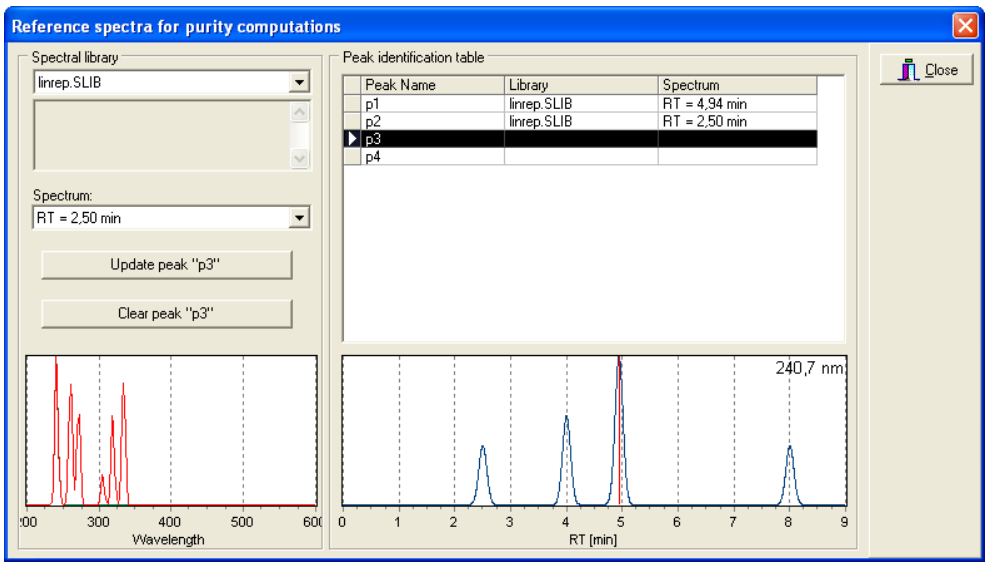
- 50% Peak Height Method: uses the spectrum extracted at 50% of peak height. This measurement is not affected by asymmetry.
- 2 Sigma Method: extracts the spectrum at 60.7% of peak height.
- 3 Sigma Method: extracts the spectrum at 32.4% of peak height.
- 4 Sigma Method: extracts the spectrum at 13.4% of peak height.
- 5 Sigma Method: extracts the spectrum at 4.4% of peak height. The five sigma method is most sensitive to asymmetry because the width is measured at the lowest point.
- 5% of Peak Height Method: extracts the spectrum at 5% of peak height.

The higher the sigma number is, the more accurate the calculation is.

In the *Purity computation* field,

1. Choose the **reference spectrum**: the spectra are compared to the peak spectrum (extract at peak apex) or to library spectra. In this case, first fill the peak identification part and then click in the peak purity part on the Ref button to choose for each spectrum, the library component.

   The following screen appears:



   In the right part of the screen the chromatogram peak names appear. A red cursor indicates in the behind chromatogram which peak is selected. For each peak, choose in the left part of the screen, the library and then the spectrum you want to use to calculate the purity. The unknown and the library spectra are displayed in the behind field respectively in red and green. The library spectrum information is displayed if you let the mouse cursor several seconds on the spectrum name. Click on the *Update peak"i"* button to calculate the purity of peak "i" with the selected library spectrum as reference. The library and spectrum names will be added in the peak identification table. Use the *Clear peak"i"* button to delete a library and a spectrum already present in the peak identification table.

Note: This peak identification table can also be filled from the result tab of the manual library search screen.

2. Choose the **Algorithm** among the 3 available algorithms (refer to The Matching Algorithms of CompassCDS section for detailed definition of the algorithms)

   Whatever the chosen algorithm, the matching factor is always between 0 (impure peak) and 1000 (pure peak).

3. Select the spectrum to be subtracted, you can select a spectrum to correct the background absorption (this background absorption can be different if the solvent is different from one analysis to another).

   Four options are available:

   - Choose **No baseline spectrum** to subtract no spectrum
   - Choose **Manual reference** to manually define the time where the spectrum must be extracted. An additional box is added behind the scrolling list where the time can be entered.
   - Choose **Peak baseline** to subtract the spectra taken at the peak start and stop. The peak start spectrum will be subtracted to spectra of the front part of the peak, e.g.. from the peak start to peak apex and the peak stop spectrum will be subtracted to spectra of the tail part of the peak, e.g., from the peak apex to peak stop. Check the *Use Spectra at Peak Start and Peak Stop* box to extract the spectrum at peak start and peak end markers. Uncheck this box to manually define the peak start and peak end times. These times can be entered in the peak identification table respectively in the RT(FBL) and RT(TBL) columns.
   - Choose **Peak baseline average** to subtract the spectrum interpolated between peak start and peak stop markers.

4. Choose the **wavelength range** for purity computations. If the *user defined* box is unchecked the purity is computed for the full acquisition wavelength range.

5. In the **Purity Thresholds** field, define the range for pure, medium or impure peaks.

   Generally, we consider that:

   A correlation superior to 990 means that peaks are similar

   A correlation between 900 and 990 represents some similarity

   A correlation inferior to 900 indicates that spectra are different.

   You can change these thresholds by modifying the values in the white fields.

6. Check **Bandwidth of average** and defined the bandwidth in the enabled field. In that case the spectra compared will be the average of spectra obtained over the defined time bandwidth.

The Peak Purity Results

The Peak Table

You can view the results of purity processing in the peak table. Select report properties in the peak table pop-up menu and then choose the purity variables you want to display. The following screen shows the results for a search realized on seven spectra compared to the reference:

#	Name	Time [Min]	Pur(Apex)	Pur(FBL)	Pur(FH)	Pur(FL)	Pur(TBL)	Pur(TH)	Pur(TL)
1	P1_2.5 min	2,48	1000,000	0,715	857,412	244,770	63,644	999,526	987,887
2	P2_4 min	4,02	1000,000	0,583	990,529	656,083	249,483	999,635	986,749
3	P3_5 min	5,01	1000,000	1,042	970,834	863,914	161,705	989,220	962,600
4	P4_8 min	7,93	1000,000	74,991	999,299	986,776	423,829	999,786	997,720
Total									

Several variables relative to peak purity can be displayed depending of the chosen mode for purity calculations:

Pur (Apex): this variable gives the peak purity results at the peak apex. This variable is calculated whatever the purity calculation mode.

Pur (FBL): this variable gives the peak purity results at the front baseline. Be careful, this variable is calculated only if "7 spectra" or "all spectra" mode has been chosen for purity calculations.

Pur (FH): this variable gives the peak purity results at the second front peak height. Be careful, this variable is not calculated if "apex only" mode has been chosen for purity calculations. It is calculated in any other modes.

Pur (FL): this variable gives the peak purity results at the first front peak height. Be careful, this variable is calculated only if the "7 spectra" or "all spectra" mode has been chosen for purity calculations.

Pur (RL): this variable gives the peak purity results at the second tail peak height. Be careful, this variable is calculated only if the "7 spectra" or "all spectra" mode has been chosen for purity calculations.

Pur (RH): this variable gives the peak purity results at the first tail peak height. Be careful, this variable is not calculated if "apex only" mode has been chosen for purity calculations. It is calculated in any other modes.

Pur (RBL): this variable gives the peak purity results at the tail baseline. Be careful, this variable is calculated only if the "7 spectra" or "all spectra" mode has been chosen for purity calculations.

AREA_IMPURE: this variable gives the percentage of peak area which is pure. Be careful, this variable is calculated only if "all spectra" mode has been chosen for purity calculations.

AREA_PURE: this variable gives the percentage of peak area which is pure. Be careful, this variable is calculated only if "all spectra" mode has been chosen for purity calculations.

AREA_MEDIUM: this variable gives the percentage of peak area which is pure. Be careful, this variable is calculated only if "all spectra" mode has been chosen for purity calculations.

This table can then be printed. The report style must contain a peak table object which format contains the chosen variables (see CompassCDS Report Editor for more details).

The Ratio Chromatogram

Purity of peaks can also be represented by the Ratio Chromatogram. The absorbance ratio of two wavelengths over time is plotted (it is the ratio chromatogram). If the ratio does not change over time a peak is considered to result from a single compound. Otherwise, the peak is considered to result from several compounds.

To build a ratio chromatogram:

1. In the peak purity subsection of an extracted chromatogram, check the *Ratio Chromatogram* box.
2. Enter the *reference wavelength*. The ratio chromatogram is the ratio of the reference wavelength absorbances by the extracted chromatogram wavelength absorbances.
3. Enter a *threshold*. At each time, if the height of the peak is lower than that threshold, the ratio will be set to zero.

Ratio Chromatograms can be displayed as other Peak Purity results.

The Peak Purity Display (the peak properties)

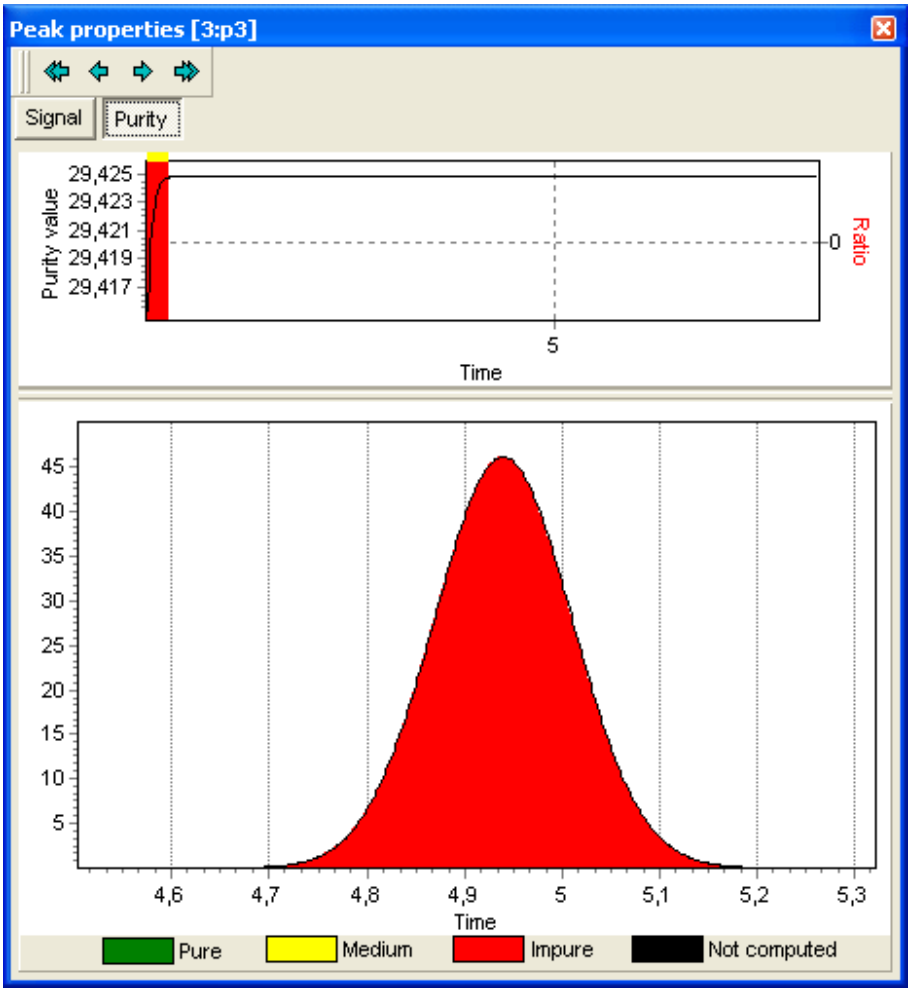
CompassCDS allows visualizing, directly on the peak, area of peak which is pure, impure or medium, a graph relating the peak purity versus the time and the Ratio Chromatogram if any.

When using the method comparing all the spectra (choose *all spectra* in the *number of extracted spectra* scrolling list of the *spectra selection* area), the correlation is calculated at each acquisition point of the peak.

Therefore, each point belongs to one of the three correlation value domains:

- High purity
- Medium purity
- Impurity represented by a lack of correlation

Click on the peak properties icon ( ) and then go in the **Purity** tab. The following screen appears:



On the top part of the screen, the ratio chromatogram and the purity values are displayed. (A graph relating the variation of the purity versus time is also given for each peak. If ratio chromatograms have been defined, the ratio is also displayed here.).

On the bottom part of the screen, the peak purity is displayed in color and the segments of co-elution are instantaneously identified. Click on , , , respectively to display the next peak, the previous peak, the last peak and the first one.

In the case of a comparison not realized on all spectra, each point used for the computation belongs to one of the three correlation value domains. All the other points are displayed in black (Not computed) in the peak properties.

These results can then be printed. The report style must contain a peak purity object (see CompassCDS Report Editor for more details).

The Matching Algorithms of CompassCDS

The correlation method

$$\text{Matching factor} = 1000 \times \frac{\left(\sum_n a_1.a_2 - \frac{\sum_n a_1 \sum_n a_2}{n} \right)^2}{\left(\sum_n a_1^2 - \frac{\left(\sum_n a_1 \right)^2}{n} \right)\left(\sum_n a_2^2 - \frac{\left(\sum_n a_2 \right)^2}{n} \right)}$$

a1 and a2 are the absorbance of the unknown and the reference spectra, measured at the same wavelength.

n: number of point acquired by spectra

Note that Matching Factor = 0 if

$$\sum_n a_1^2 - \frac{\left(\sum_n a_1 \right)^2}{n} = 0 \quad \text{or} \quad \sum_n a_2^2 - \frac{\left(\sum_n a_2 \right)^2}{n} = 0$$

The similarity method

$$\text{Matching Factor} = 1000 \times \frac{\sum_n a_1 a_2}{SQRT\left(\sum_n a_1^{\,2} \times \sum_n a_2^{\,2} \right)}$$

a_1 and a_2 are the absorbance of the unknown and the reference spectra, measured at the same wavelength.

n: number of point acquired by spectra

The dissimilarity method

$$\text{Matching Factor} = 1000 \left(1 - SQRT\left(1 - \frac{\left(\sum_n a_1 a_2 \right)^2}{\sum_n a_1^{\,2} \times \sum_n a_2^{\,2}} \right) \right)$$

a_1 and a_2 are the absorbance of the unknown and the reference spectra, measured at the same wavelength.

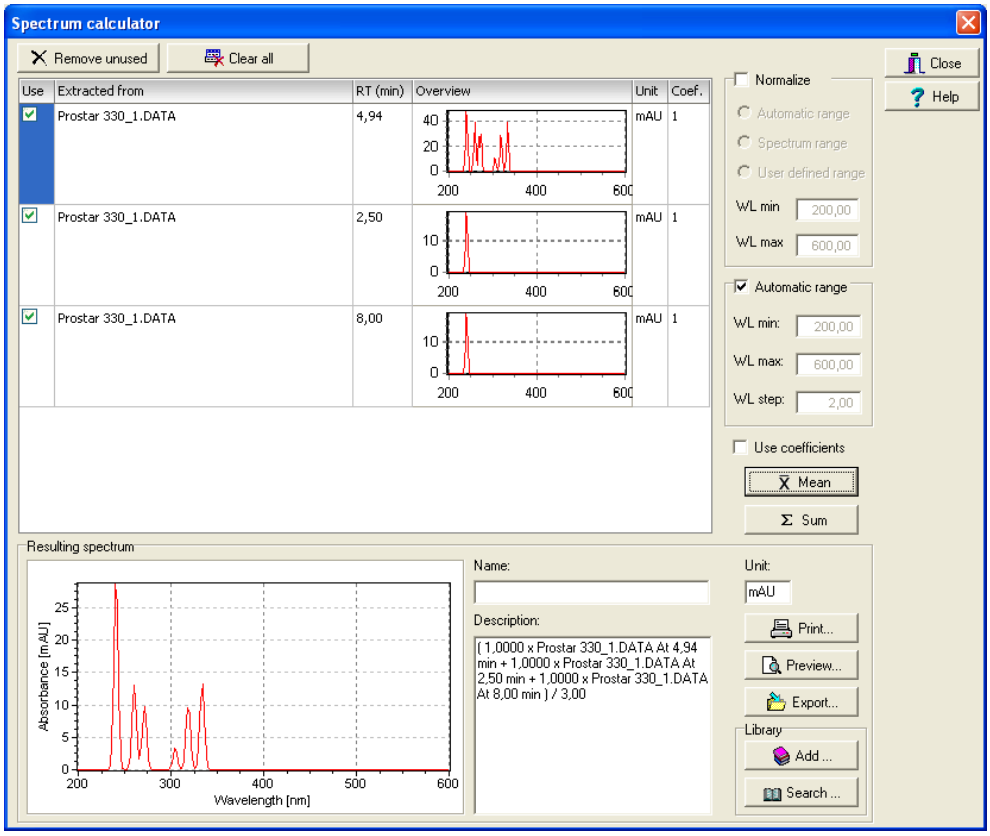
n: number of point acquired by spectra

The Spectrum Calculator

The Spectrum Calculator allows the calculations to be performed (additions and subtractions) on spectra.

To select the spectra you want to perform calculations on, choose 'spectrum processing' then 'send spectrum to calculator' from the pop-up menu in the spectrum window of the 4-view mode or press the "*to calculator*" button from a spectral library.

To open the Spectrum Calculator, click on the button in the CompassCDS toolbar. The following screen appears:



The Spectrum Calculator window is composed of 3 parts: the spectrum list, the parameters settings, and the resulting spectrum part.

The Spectrum List

In the spectrum list, all the selected spectra are displayed with their names, retention times, overviews and the units of the response. All those fields are in read-only mode. In the last column, the coefficient that will be used for the calculations can be set.

Parameters Settings

On the right part of the window, the normalization and computation parameters can be set.

The normalization can be inactive or be set to automatic, spectrum or user defined wavelength range.

- **Automatic range**: all spectra are normalized in the common wavelength range.
- **Spectrum range**: each spectra is normalized in its own wavelength range.
- **User defined range**: all spectra will be normalized in the wavelength range defined by the user.

The computation can be performed on the total wavelength range of the acquisition if the automatic option is checked, or on a user defined range. If the chromatograms have different acquisition wavelength ranges, the calculations will be done on the common range only. The step used for the computation can also be set.

Two actions can be done: 'sum' or 'mean'.

- The **'sum'** option sums all the selected chromatograms, taking each coefficient into account if the "use coefficient" box is checked.
- The **'mean'** action sums all the selected chromatograms, taking each coefficient into account if the "use coefficient" box is checked, and divide it by the sum of coefficient.

Resulting Spectrum

On the bottom of the window, the resulting spectrum is displayed. A name, the unit of the response and a description can be edited.

The resulting spectrum can be previewed and printed (using a report style previously created), exported or added to a spectral library.

A search in library can also be performed to compare this calculated spectrum with reference ones.

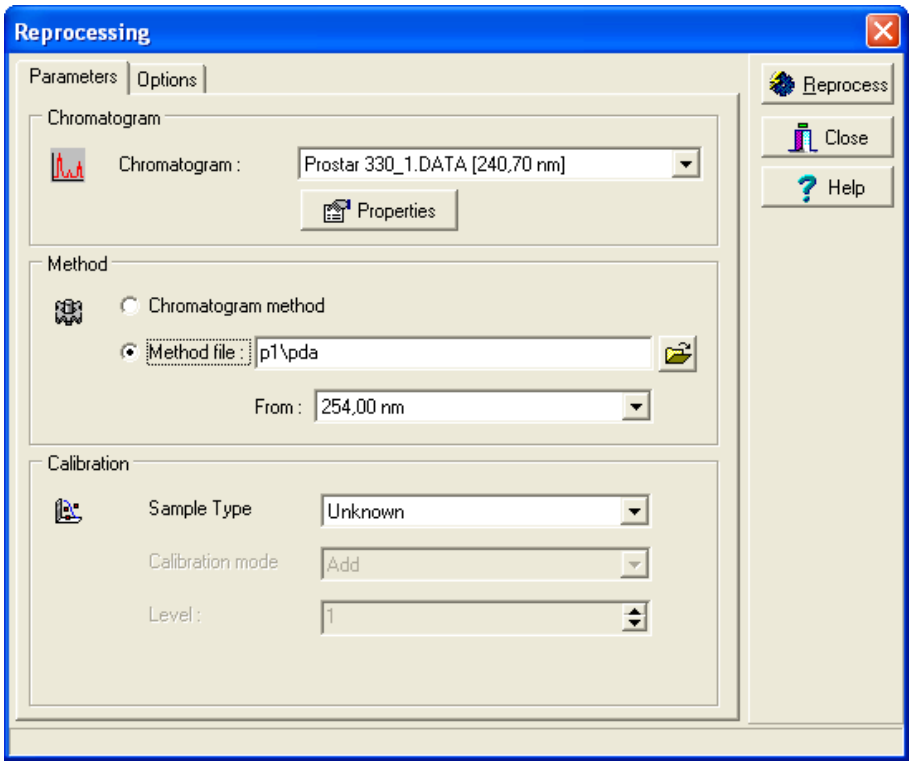
Reprocess the PDA Chromatogram

Once a chromatogram has been acquired, it is possible to reprocess it with another method.

Single Reprocessing

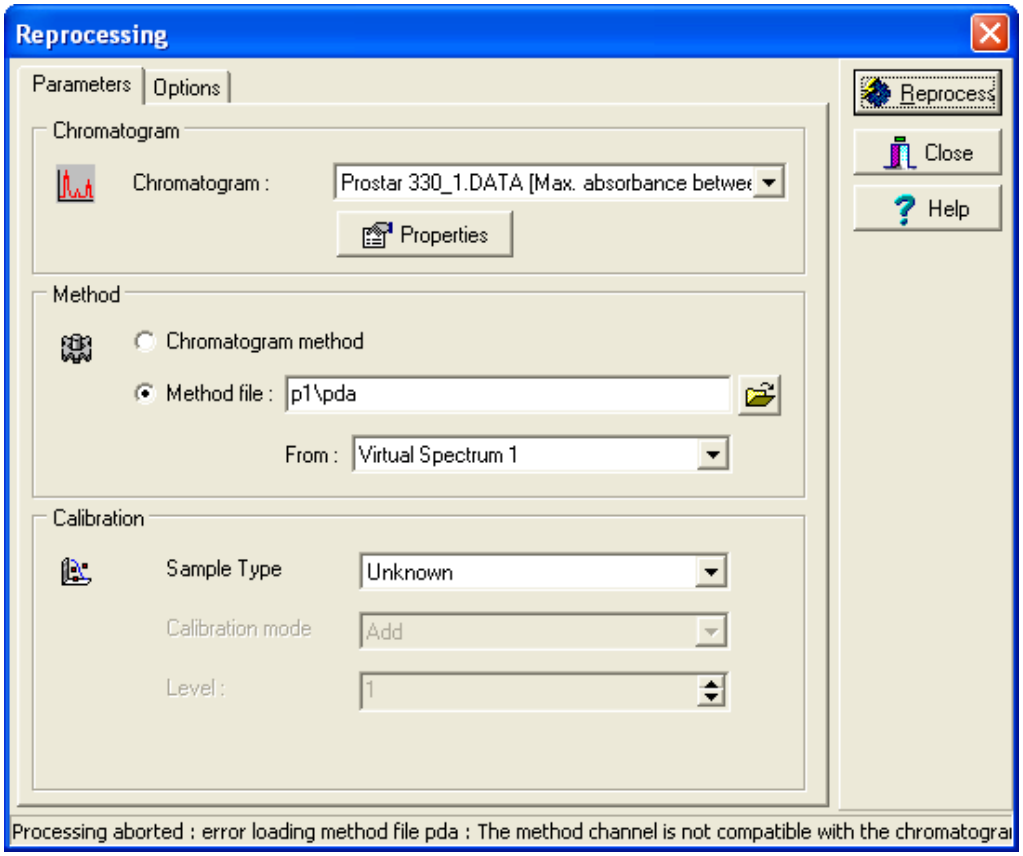
The chromatogram should be opened in CompassCDS to be reprocessed in the single reprocessing window.

Choose the menu *PROCESSING / REPROCESSING / ACQUISITION* to access the reprocessing window (or click on F6, or press the button):



In the Chromatogram zone, select the chromatogram file to reprocess from the list of all the chromatogram names opened in CompassCDS. Choose the right one then choose the method in the corresponding zone. If ‘Chromatogram method’ is chosen, the method inside the chromatogram file is used. If another method has to be used, choose ‘Method file’ to access the open file window to choose the name of the method, and press the open icon ( ).

Be careful to choose the right channel of the chromatogram and the right channel of the method. If they are not compatible (for example if the spectrum channel has been chosen for the chromatogram and an extracted channel for the method) a message will be displayed in the bottom of the screen as follows:



Note: If the chromatogram already contains extracted channels and is reprocessed with a method which contains other extracted channels, all the channels will be added.

If the chromatogram and the method used for reprocessing contain the same extracted channel, the chromatogram will be modified according to the method.

Reprocessing Multiple Chromatograms (Reprocessing List)

To quickly reprocess multiple chromatograms, it is possible to create a reprocessing list:

Select the menu FILE / NEW / NEW REPROCESSING LIST. (Refer to the CompassCDS User Guide to learn how to create a reprocessing list).

The columns of the reprocessing list are very similar to the column of the sequence:

In the “Chromatogram name” column, select the name of the chromatogram(s) to be reprocessed.

In the “Chromatogram channel” column, select the chromatogram channels that should be processed. For example, to reprocess one of two channels, select in this box the name of the channel to reprocess.

In the Method name, select the name of the method to apply. In the method channel, select which method channel should be applied if the method is defined for more than one channel.

Note: If the chromatogram already contains extracted channels and is reprocessed with a method which contains other extracted channels, all the channels will be added.

If the chromatogram and the method used for reprocessing contain the same extracted channel, the chromatogram will be modified according to the method.

Index

3D method, 9
3D variables, 12
Acquisition, 14
Baseline monitoring, 14
Chromatogram, 58
Chromatogram extraction, 10
Extracted chromatogram, 12
Label, 39, 46
Maximum absorbance chromatogram, 18, 36
PDA displaying, 26
Peak purity
  Parameters, 54
  Results, 57
Ratio chromatogram, 58
Reprocess, 62
Spectral library
  New, 41
  Open, 43
  Search, 48

CompassCDS Configuration Manager User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501482
Revision D

Contents

Using CompassCDS Configuration Manager 3
What is the CompassCDS Configuration Manager? 3
Software Function 3
Logging into CompassCDS Configuration Manager 3
Main Screen Architecture 4
Organization Tab 8
CompassCDS Configuration Manager Organization 13
The Organization Items 13
The Stations / Systems Items 33
Organization Configuration (Items Associations) 42
Connections 44
Tools 45
Configuration Parameters 45
Security 46
Password 47
Audit Trail 53
Current Audit Trail Viewing 53
Archived Audit Trail Viewing 55
Audit Trail Query 56
Configuration of Audit Trail content 61
Reason configuration 61
Options 62
Licenses 62
Devices 63
Lock Connection 63
View 63
Refresh 63
Show Console 63
Show Properties 64
Groups 64
Projects 65
Users 65
User profiles 65
Admin profiles 65
Stations 65
Systems 65
Connections 65
File 65
Preferences 65
Quit 66
Help 66
Help 66
About 66
CompassCDS File Management under Windows 66
Glossary 68

Using CompassCDS Configuration Manager

This document describes the functions of the CompassCDS Configuration Manager.

What is the CompassCDS Configuration Manager?

The CompassCDS Configuration Manager is the software interface between System Administrators and the Main Server & Acquisition Server modules of CompassCDS. This application provides the means to create and configure Groups, Projects, Users and Systems as well as to maintain detailed logs of information regarding system activity and security.

CompassCDS Configuration Manager is installed as part of CompassCDS.

Before starting it is recommended that users examine the Glossary on page 68 to become familiar with the terminology used within this guide.

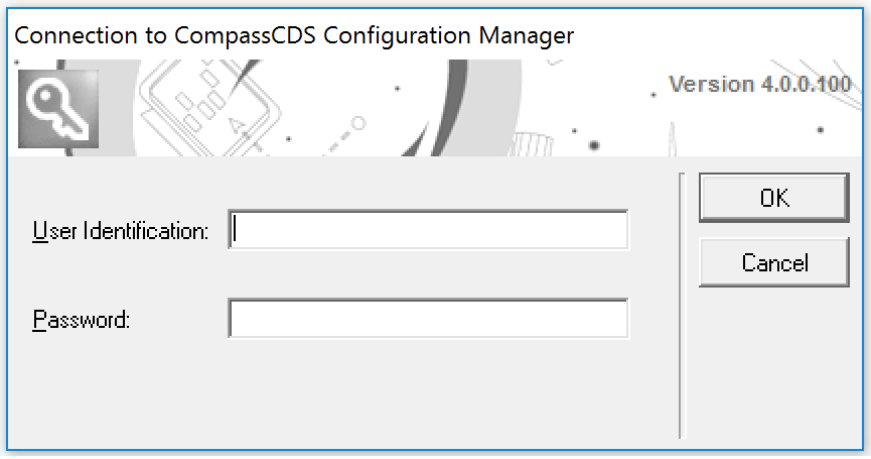
Software Function

Logging into CompassCDS Configuration Manager

Run the CompassCDS Configuration Manager from Windows Start Menu → Programs→ CompassCDS (Chromatography System) → CompassCDS Configuration Manager, or double click on the corresponding desktop icon.

When the logon window appears, type *admin* in User Identification field and *compass* in the Password field. After logging into the CompassCDS Configuration Manager, it is possible to change the administrator logon. Any user that has been assigned administrator rights (see New/Edit user section) can log into the CompassCDS Configuration Manager with his/her name and password.

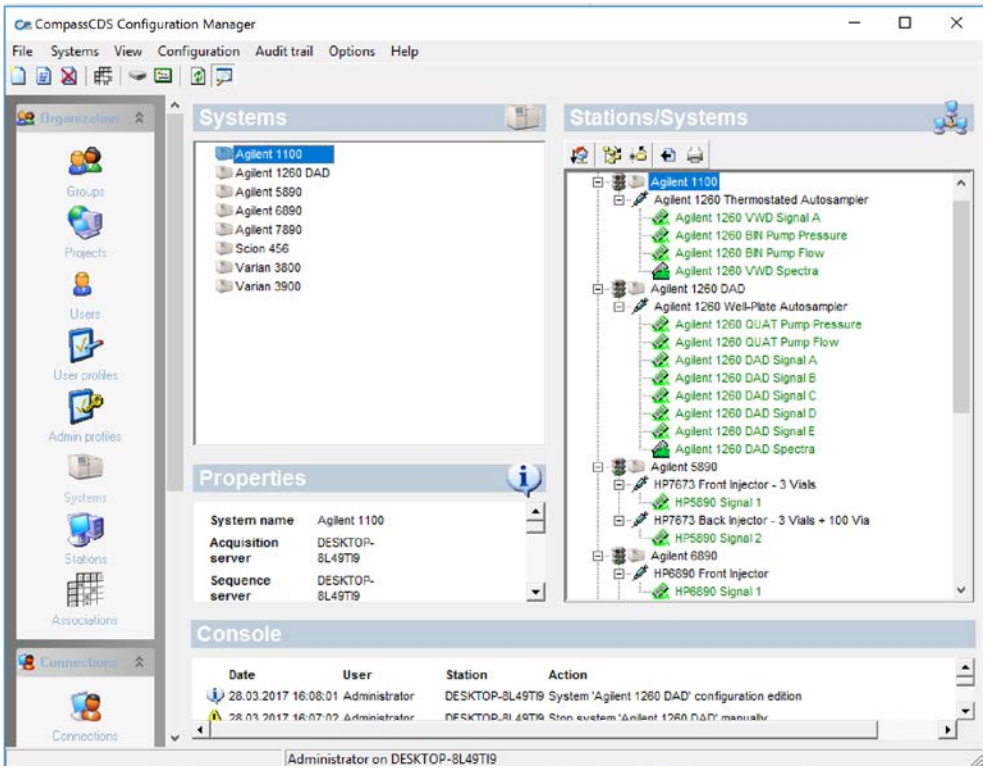
The password is case sensitive (abc ≠ ABC).



Main Screen Architecture

The main window is divided into:

- A browser (on the left) and one or three panels depending upon the type of information selected in the browser which has three sections (Organization, Connections, and Tools). Popup menus are available within the panels.



- A menu bar allows access to configuration parameters, audit trail options, etc. and is made up of the following options:

File:

Preferences: Used to configure user dependent display parameters..

Quit: To exit the CompassCDS Configuration Manager.

Groups/ Projects/ Users/ User profiles/ Admin profiles/ Stations/ Systems:

The title of this menu changes depending on which item is selected in the organization table.

New: To create a new item.

Edit: To display the editable properties of the selected item.

Delete: To delete the selected item.

Duplicate: To duplicate the selected item.

Export list: To export a list of the selected item.

Export properties: To export the properties of the selected item.

Print list: To print the selected item list.

Print properties: To print the properties of the selected item.

View:

Refresh: To refresh the database.

Show console: To turn the console display on or off.

Show properties: To turn the properties screen display on or off.

Groups: To directly display the Groups list.

Projects: To directly display the Projects list.

Users: To directly display the Users list.

User profiles: To directly display the User profiles list.

Admin profiles: To directly display the Admin profiles list.

Stations: To directly display the Stations list.

Systems: To directly display the Systems list.

Connections: To directly display the Connections screen.

Configuration:

Associations: To access the screen that allows an administrator to define links between items: associations of Groups / Projects / Users / User profiles, Systems and Paths definition (see page 42).

Security: To define the security parameters: lock user account, lock session, etc. (see page 46).

Password: To define the password configuration parameters: minimal length, expiration, history (see page 47).

Electronic signature: To configure electronic signature parameters (see page 49).

Parameters: To configure certain general parameters: calibration curve orientation, message of the day, etc.

Audit trail:

Current audit trail: To display the current audit trail (see page 53).

Audit trail archives: To display an archived audit trail (see page 55).

Configure audit trail: To select the actions to log in the audit trail (see page 61).

Configure reasons: To define the reasons that can be selected by users when changes are made either within the CompassCDS Configuration Manager or the CompassCDS Chromatography Data System (see page 61).

Tools:

Devices: To access the screen that enables instrument drivers to be manually updated (access reserved for Scion Instruments service engineers).

License: To access the license manager module to manually input additional license serial numbers.

Help:

Help: To access the on-line help.

About: To access the software information screen.

- The Configuration Manager also has an icon bar that enables rapid access to functions listed in the menu bar.

: Creates a new item.

: Edits the properties of a selected item.

: Deletes the selected item.

: Access the screen that enables an administrator to create and modify links between items: associations of Groups/ Projects/ Users/ User profiles/ Systems and Paths definition.

: Displays the current audit trail.

: Displays an archived audit trail.

: Accesses the license manager.

: Refreshes the database.

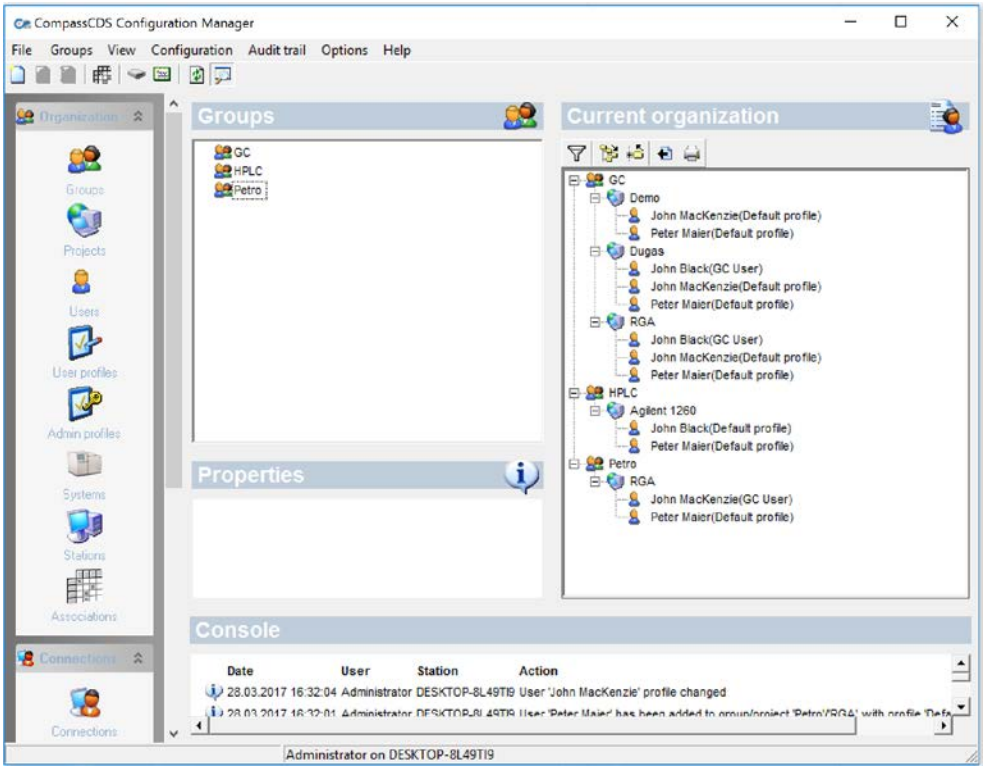
: Toggles the console display on or off.

- Configuration Manager also has a task bar that indicates the name of the connected administrator and name of the computer station.
- Configuration Manager also has a list of Shortcuts that enable access to certain functions.

Action	Shortcut
Display User list	Alt+1
Display Project list	Alt+2
Display Group list	Alt+3
Display User profile list	Alt+4
Display Admin profile list	Alt+5
Display System list	Alt+6
Display Station list	Alt+7
Display Connections	Alt+8

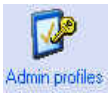
Action	Shortcut
Display Tools	Alt+9
Create a new item	Insert
Display all connections of the selected item	F7
Deletion of a selected item	Del
Duplication of a selected item	Ctrl+Ins
Display Preferences	F2
Exit application	Alt+F4
Display Organization	F6
Display Security parameters	Ctrl+Alt+5
Display Password parameters	Ctrl+Alt+6
Display Electronic signature parameters	Ctrl+Alt+7
Display Configuration parameters	Ctrl+Alt+9
Display current Audit trail	Ctrl+F5
Display Audit trail archive	Ctrl+F6
Configure reason for CompassCDS changes	Ctrl+F7
Configure reason for CompassCDS locks	Ctrl+F8
Configure reason for CompassCDS Configuration Manager changes	Ctrl+F9
Display the on line help	F1
Disconnect the selected item from its current position	Ctrl+D
Classify Stations/Systems by laboratory	F8
Stop the selected system	Ctrl+S
Start the selected system	Ctrl+R
Display properties	Ctrl+Enter
Full expansion of the tree	Ctrl+X
Full collapse of the tree	Ctrl+O
Show console	F3
Refresh the data base	F5
Export the selected list	Shift+Ctrl+E
Print the selected list	Shift+Ctrl+P
Export the tree	Ctrl+E
Print the tree	Ctrl+P
Print the properties of the selected item	Ctrl+Alt+P
Export the properties of the selected item	Ctrl+Alt+E
Display parameters to log in the audit trail list	Ctrl+Alt+8

Organization Tab



The Organization tab enables the creation and management of elements that constitute the structure of the organization (Users, Projects, Groups, User profiles, Admin profiles, Stations and Systems). These are displayed in the form of a tree which illustrates the associations between items or in the case of Stations and Systems, the associations between Laboratories/Stations/Systems. The properties and information about a selected item is also displayed.

The top left side of the window (Item lists) displays, in alphabetical order, a list of the defined items: Groups, Projects, Users, User profiles and Admin profiles, Stations and Systems. To access to an item family, an administrator selects the corresponding icon in the browser:

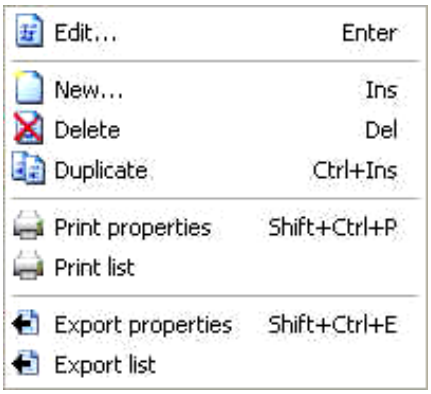
	Groups		Admin profiles
	Projects		Stations
	Users		Systems
	User profiles		Associations

In the Item lists, some item names can be preceded by a symbol to notify the connected administrator of the state of that particular item. These symbols are explained in the following table:

Item	Symbol	Meaning

User		Is an administrator
		User account locked
		User account deactivated
User profile		Is the default user profile
Admin profile		Is the default admin profile
Station		Is locked
		Is an acquisition server
System		Is locked

When an administrator right-clicks on an item, the following menu for that item is displayed.



Edit: opens the properties screen of the item for editing.

New: creates a new item.

Delete: Deletes the selected item(s). The Ctrl or Shift keys can be used to select several items in the list.

Duplicate: Duplicates the selected items. The Ctrl or Shift keys can be used to select several items in the list. The name of the duplicated item is prefixed with “Copy of”. In the case of the duplication of a User, the User ID is also prefixed with “Copy of” User ID and no password is defined by default.

NOTE: The duplication of Group, Project or User causes the creation of associations (Group/Project/User/User profile); a message advises the administrator to change the path if necessary. By default the same Group or Project path or User path is retained.

Export properties: Exports the properties of the selected item(s). In the case of multi the selection of multiple items, the information concerning all the selected items is exported in the same file. The export format is HTML.

Export list: Exports the list of the item(s) displayed on the screen. The export format is HTML.

Print properties: Prints the properties of the selected item(s). When multiple items are selected, the properties of all the selected items are printed.

Print list: Prints the list of the item(s) displayed on the screen.

When the item list is right clicked without any items being selected, a general popup menu is displayed. This menu has only the New, Print list, and Export list commands active.

The bottom left side of the window displays the properties of the item selected in an item list, or the information of the item selected in the right screen: *Current organization.*

The properties screen displays the parameters relative to the item selected in the Item list, whereas the information screen displays information on the item selected in the current organization and relative to the current association.

For example:

Item list: Creation of a new user.	**Properties :**
User name: John Doe	User name: John Doe
User ID: John	User ID: John
Initials: JD	Initials: JD
Password: john123	Password defined
E-mail address: jd@Scion Instruments.com	E-mail address: jd@Scion Instruments.com
Description: chemist	Description: chemist
User account: activated	User account: activated
Administrator with profile default_admin	Is an administrator Admin. Profile: default_admin
Can log on all my projects with profile profile1	Can log on all my projects with profile profile1
Allowed to work on Station1	Allowed stations: Station1
Associated to group1/p1 (path: C:\CompassCDS\Data\p1 and profile: default_profile).	Associated groups/projects: group1/p1
Current organization :	**Information :**
Select John Doe in the tree	Group name: group1 Project name: p1 User name: John Doe User ID: John Log on all projects with profile: profile1 Current path: C:\CompassCDS\Data\p1 Profile: default_profile Allowed stations: Station1

The right side of the window displays the Current organization which shows, in the form of a tree, a clear overview of the associations between Groups / Projects / Users / User profiles.

The following icon bar is available and it enables administrators to**:**

display only connections of the item selected in the Item list.

expand the tree.

reduce the tree.

export the tree.

print the tree.

When an administrator right-clicks on a Project or a User, a pop-up menu, this enables the removal of a Project and its associated Users from a Group, or the Removal of a User from a Project, appears.

When Stations or Systems are selected in the Organization tab, the right side of the window displays Stations/Systems organization in the form of a tree that provides a clear overview of the associations between Laboratories / Stations / Systems.

An icon bar is available: . It allows an administrator to:

classify Station / Systems by Laboratory, if any defined.

expand the tree.

reduce the tree.

export the tree.

print the tree.

When an administrator right-clicks on a system (if the connected administrator owns the corresponding right), a menu pops up that allows the system to be stopped or started. This function can be useful in cases when communication problems with a system occur.

NOTE: When selecting an item in the corresponding item list, it is displayed on a colored background, both in the item list and in the Current organization or Stations/systems screens, to show its association(s).

CompassCDS Configuration Manager Organization

The Organization Items

The Group

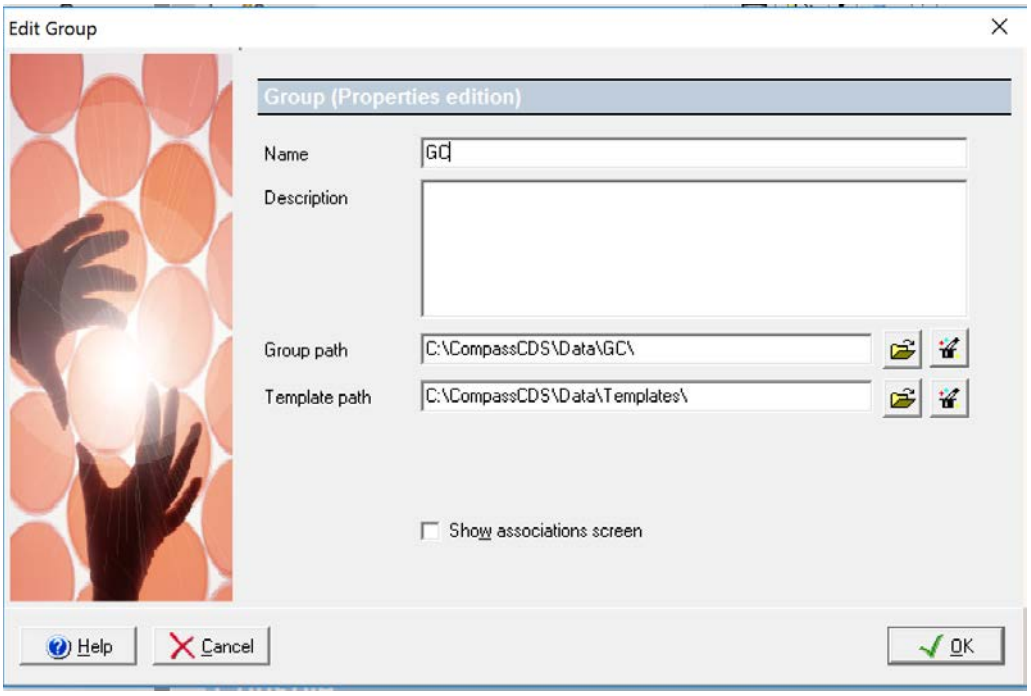
The group represents the first level in the Configuration Manager directory structure.

To display the group parameters, select the

icon in the organization browser.

Creating a Group

Right-click in the *Groups* panel, and select the *NEW* option in the popup menu, or select the *GROUPS/ NEW* menu option.



The Group properties wizard appears:

Enter the Group name (40 characters maximum), a description (255 characters maximum), (optional), the Group Path and the Template path. The group path is used to locate chromatographic data, methods, etc. The Template path defines the directory where the template methods are saved (See the CompassCDS Chromatography Data System User's Guide to learn more about the templates utility).

It is important to have a well-defined group path. All projects that are members of this group will automatically have a project path that is a subdirectory of this group data path.

NOTE: It is possible to define a group path that consists of a mapped network drive.

The Show associations screen checkbox causes the Associations screen to be displayed when this wizard is closed.

The group with displayed information is created by clicking the *OK* button.

Editing a Group

Any information concerning a particular group can be modified by double clicking on the group name, or selecting the *Edit* option in the group popup menu to access the properties screen.

The Project

The Project is the second level in the Configuration Manager directory structure.

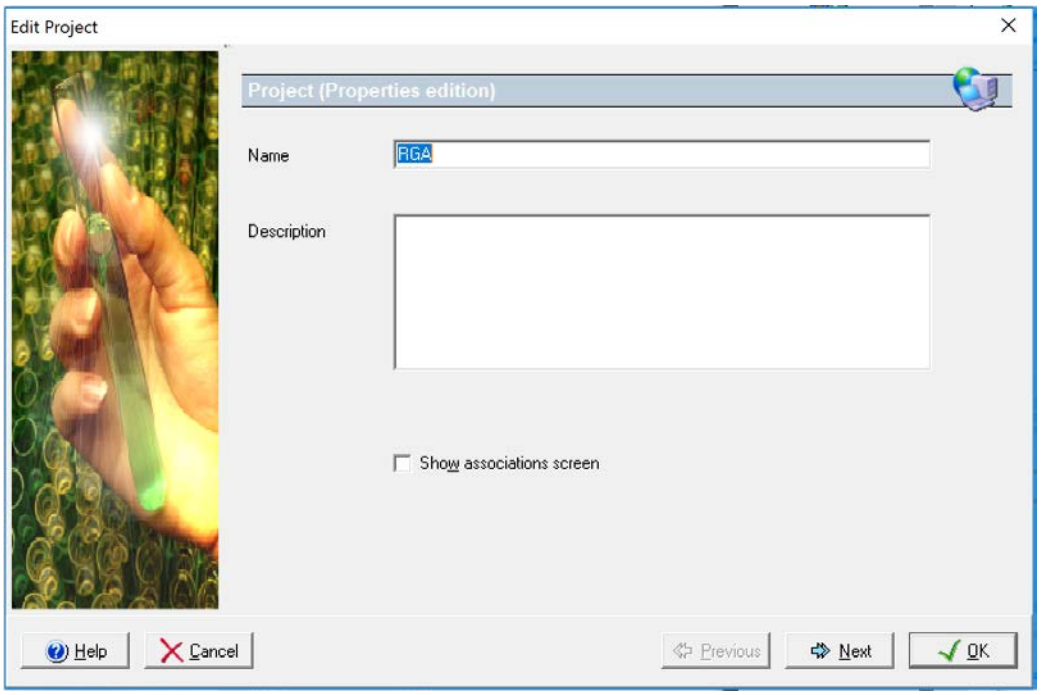
To display the Project parameters, select the

icon in the Organization browser.

Creating a Project

Right-click in the *Projects* panel, and select the *NEW* option in the popup menu, or select the *PROJECTS / NEW* menu.

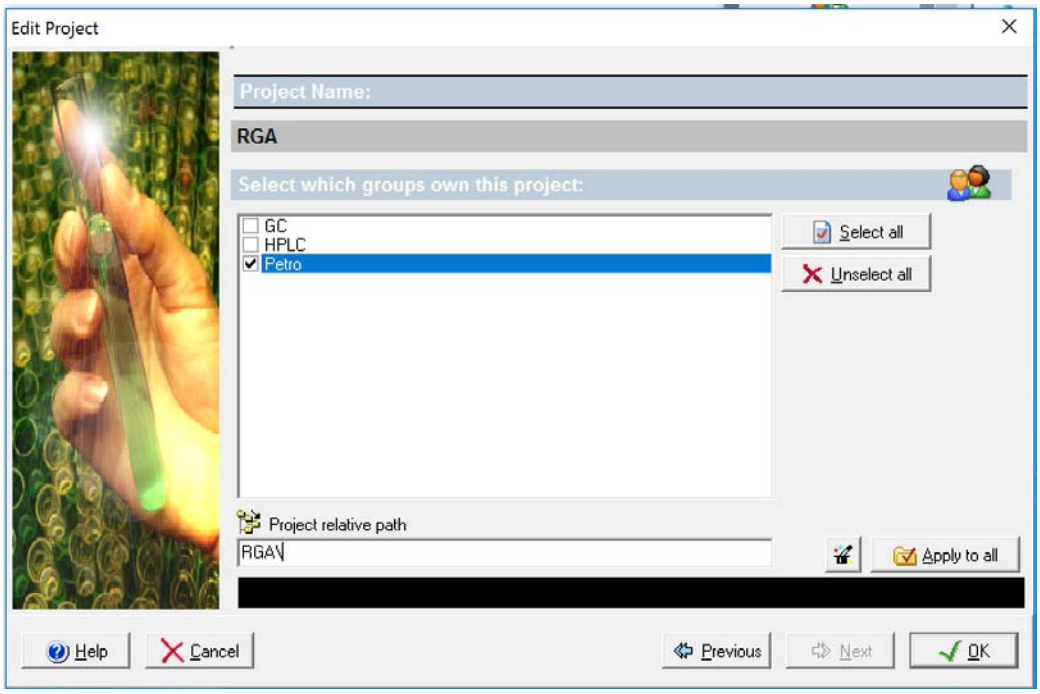
The Project properties wizard will appear:



Enter the Project name (40 characters maximum), and a Description (255 characters maximum, optional).

Checking the Show associations screen checkbox causes the Associations screen to be displayed when this wizard is closed.

Press the *Next* button to display the second screen:



It is possible to select the group(s) to which the project will be directly associated, in this screen. Once a project is associated to a group, the *project relative path* is activated, and this enables the administrator to define paths. To automatically add the name of the project in the *Project relative path* field, click on the button. To apply the relative path of this project to all the checked group/project associations, click on the Apply to all button.

To associate in a single step the project to all the defined groups, click the Select all button.

To remove in a single step the project from all the defined groups, click the Unselect all button.

The project is then created, with the displayed information, by pressing the OK button.

Editing a Project

Any information concerning a particular project can be modified by double clicking on the project name, or selecting the *Edit* option in the project popup menu to access the properties screen.

The User

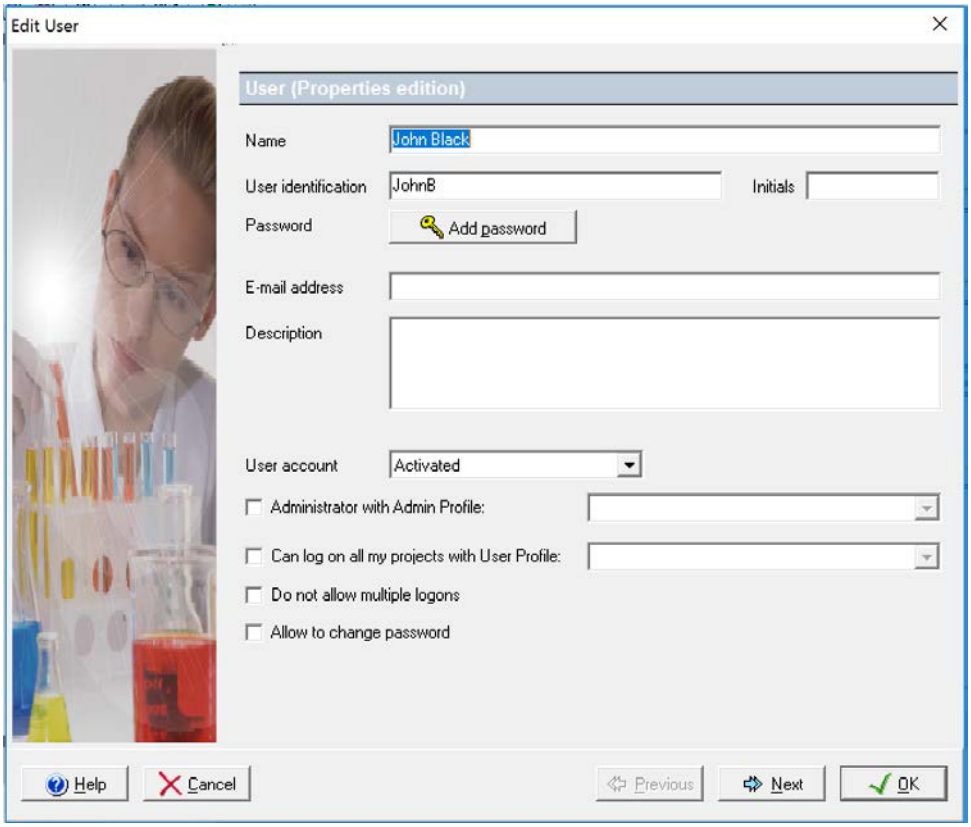
The user represents the user of the software. User can be considered the third level in the Configuration Manager Directory structure, as a path can be defined by user name to store data.

To display the user parameters, select the Users icon in the organization browser.

Creating a User

Right click in the *Users* panel, and select the *NEW* option in the popup menu, or select the *USERS / NEW* menu.

The User properties wizard will appear:



The following information fields need to be completed

Name: This is an informative field which appears everywhere on the CompassCDS reports where the Operator name is specified. This field is mandatory and must be unique within the CompassCDS Configuration Manager Database (40 characters maximum).

User ID: This is the user name entered in the logon box of CompassCDS (31 characters maximum). This field is mandatory, and needs to be unique within the CompassCDS Configuration Manager Database.

Initials: Initials are used by certain variables within CompassCDS to, for example, generate a data filename prefix or to save chromatograms in a directory corresponding to the user name (See the Tokens section in user profiles). This field is optional (4 characters maximum).

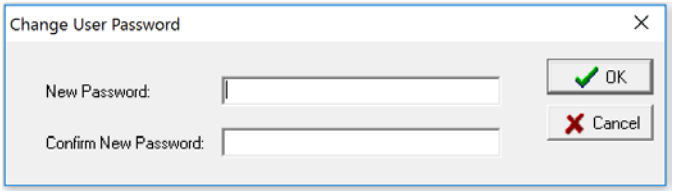
Password: Enter a password (40 characters maximum). This field is only mandatory if the administrator forces users to have a password (see the section dealing with password configuration).

Passwords are case sensitive, meaning that abc ≠ ABC. It is possible to use any of the ASCII characters to create a password.

To change a password, an administrator clicks on the

icon.

The following screen will be displayed:



The Administrator either enters a new password for the selected User (if the user has no rights to modify his/her password), or a temporary password (if the user has rights to modify his/her password) and then has to confirm it.

E-mail address: Defines the e-mail address of the user (100 characters maximum).

Description: Enables an administrator to enter any comments about the user (255 characters maximum). This field is optional.

User Account: This field is used to temporarily lock/unlock a user account in order to deactivate or to activate him/her. If a user account is locked, the user will be unable to connect to CompassCDS and the user name will be preceded by a padlock in the Item list in the top browser. When a user account is deactivated, this user is removed from all group/projects in the Organization view and from the organize screen but it is still listed in the list of users.

Administrator with profile...: This field is checked to provide CompassCDS Configuration Manager access permission to a user by making this user a member of the Administrator group. An admin profile must be selected in the associated scrolling list, to define the rights of this administrator in the CompassCDS Configuration Manager. By default the *Default admin profile* is selected.

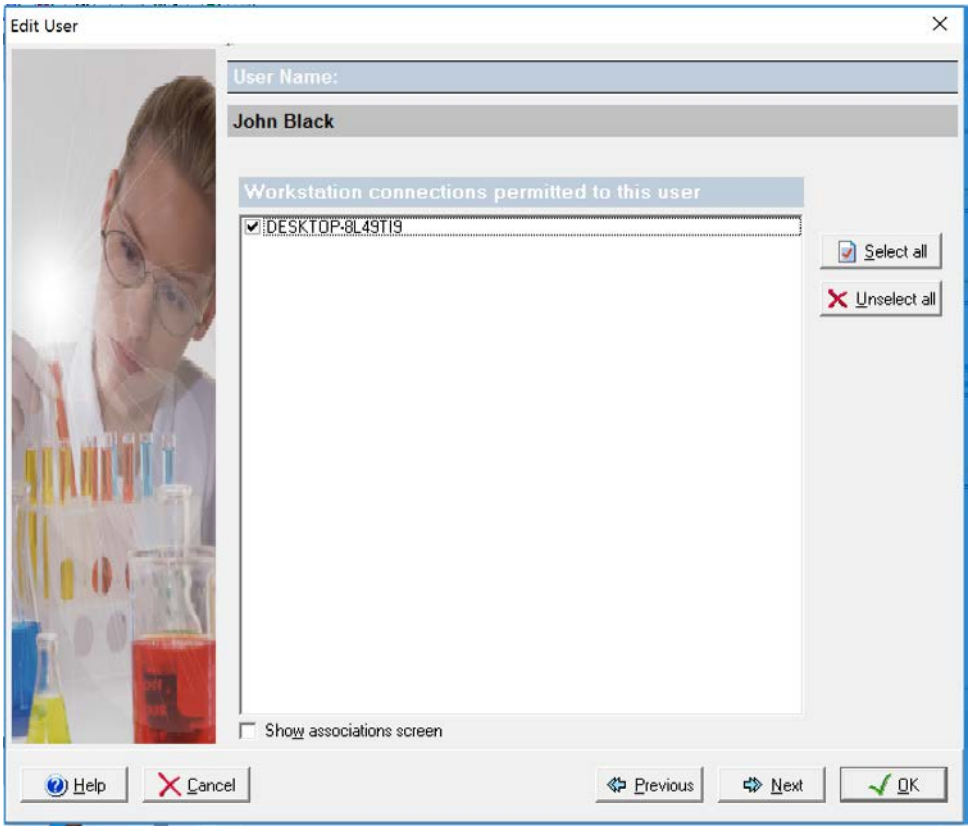
NOTE: It is possible to create administrators with unique profiles that have different levels of permissions.

Can log on all my projects with profile...: This field is checked to provide the user the right to connect to a group folder within CompassCDS and not just to within in a group / project folder. This enables user to access all the projects associated with a particular group in the same session. A User profile must be selected in the associated scrolling list, to define the rights of this user in CompassCDS. By default the *Default user profile* is selected.

Do not allow multiple logons: Checking this field prevents the user from connecting to more than one CompassCDS session at a time.

Allow to change password: Checking this field enables the user to change the password from within an active CompassCDS session.

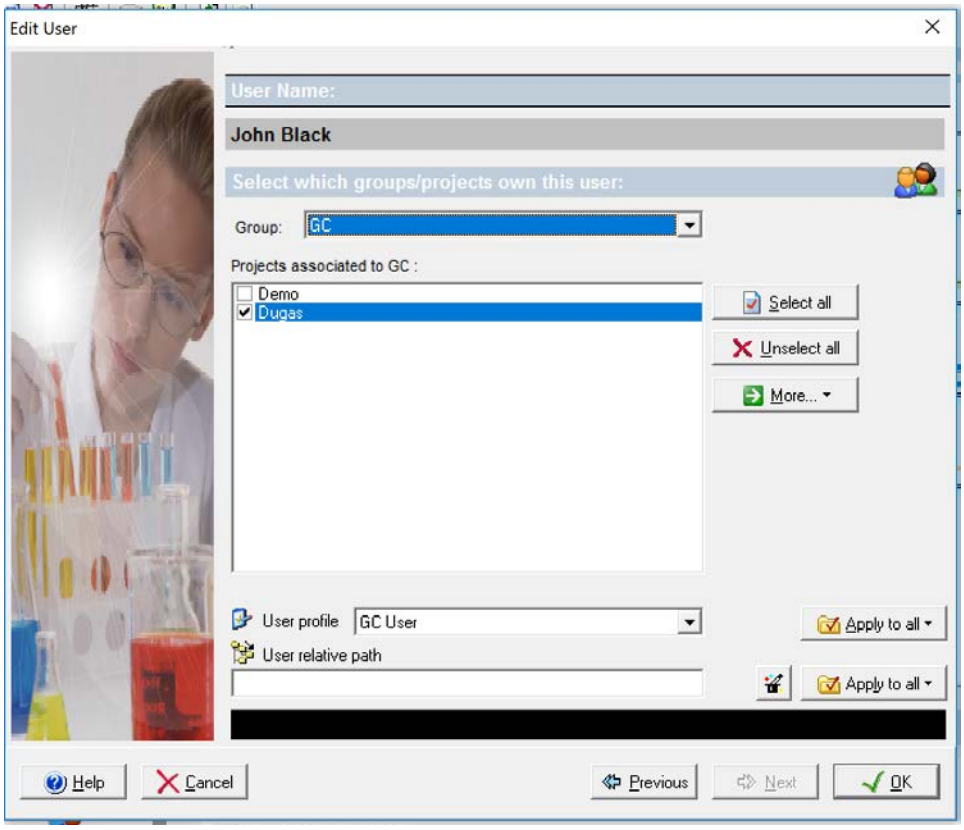
Once these fields have been completed, clicking on the *Next* button displays the following screen:



In this screen, the stations (CompassCDS client computers) that the user is authorized to connect to can be selected by an administrator.

The Show associations screen checkbox causes the Associations screen to be displayed when this wizard is closed.

Pressing the *Next* button displays the third screen:



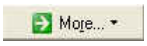
It is possible to select the group(s) and then the project(s) to which the user will be directly associated in this screen. Once a user is associated to a group/project, the *user profile* and the *user relative path* fields are activated, allowing the administrator to define both the user profile and the user relative path (optional).

Clicking the

button associates the user to all the projects of a group in a single step.

Clicking the

button removes the user from all projects of a group in a single step.

Clicking the 

button associates the user with a selected project in all groups. Select the *Associate to 'project name' in all groups'* option. To remove the user from the selected project in all groups, select the *Remove from 'project name' in all groups'* option.

Clicking the

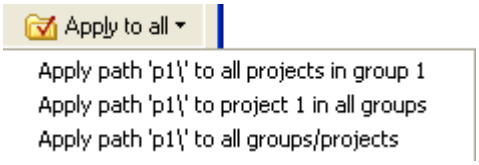
button associates the user with all the existing group/project associations. Select the *Associate to all groups/projects* option. To remove the user from all defined groups/projects, select the *Remove from all groups/projects* option.

Filling the *Path* and *User profile* fields automatically:

To automatically add the name of the user in the *User relative path* field, click on the
button.

To apply the relative path of this user to all the projects associated to the selected group, click on the

button. Clicking on the arrow provides several options:


Apply to all
Apply path 'p1\' to all projects in group 1
Apply path 'p1\' to project 1 in all groups
Apply path 'p1\' to all groups/projects

The *Apply path 'X' to all projects in 'group name'* leads to the same action, as selecting, *Apply to all would*.

To apply this user relative path to a specific project in all the defined groups, select the *Apply path 'X' to 'the selected project' in all groups'* option.

To apply this user relative path to all the existing groups/projects, select the *Apply path 'X' to all groups/projects* option.

To apply the user profile of the selected user to all the projects associated to the selected group, click on the

button. Clicking on the arrow provides several options:

Apply to all
Apply profile Default profile to all projects in group 1
Apply profile Default profile to project 1 in all groups
Apply profile Default profile to all groups/projects

The *Apply profile 'profile name' updates all projects in 'group name'* resulting the same action as selecting *Apply to all would*.

To apply this user profile to a specific project in all defined groups, select the *Apply profile 'X' to 'project name' in all groups'* option.

To apply this user profile to all the existing groups/projects, select the *Apply profile 'profile name' to all groups/projects* option.

The user can then be created, including all the entered information, by clicking the *OK* button.

Editing a User

To modify any information concerning a particular user, an administrator can double click on the particular user name, or select the *Edit* option in the user popup menu to access the properties screen, and make the changes as needed.

The Admin Profile

The Admin profile represents the rights (permissions or privileges) given to an administrator when he/she logs in a CompassCDS Configuration Manager session.

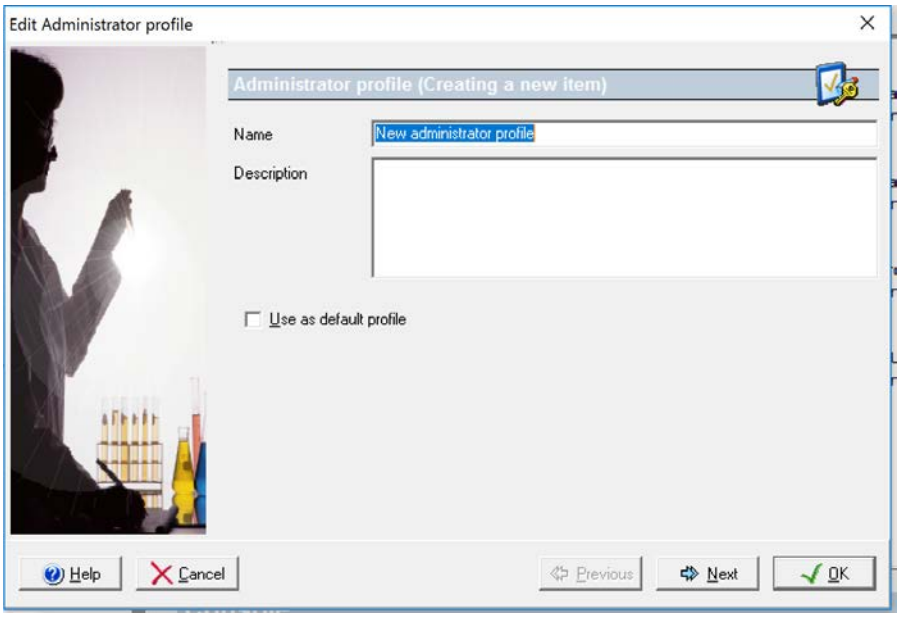
To display the Admin profile parameters, select the

icon in the organization browser.

Creating a New Admin Profile

Right click in the *Admin profiles* panel, and select the *New* option in the popup menu, or select the *ADMIN PROFILES / NEW* menu.

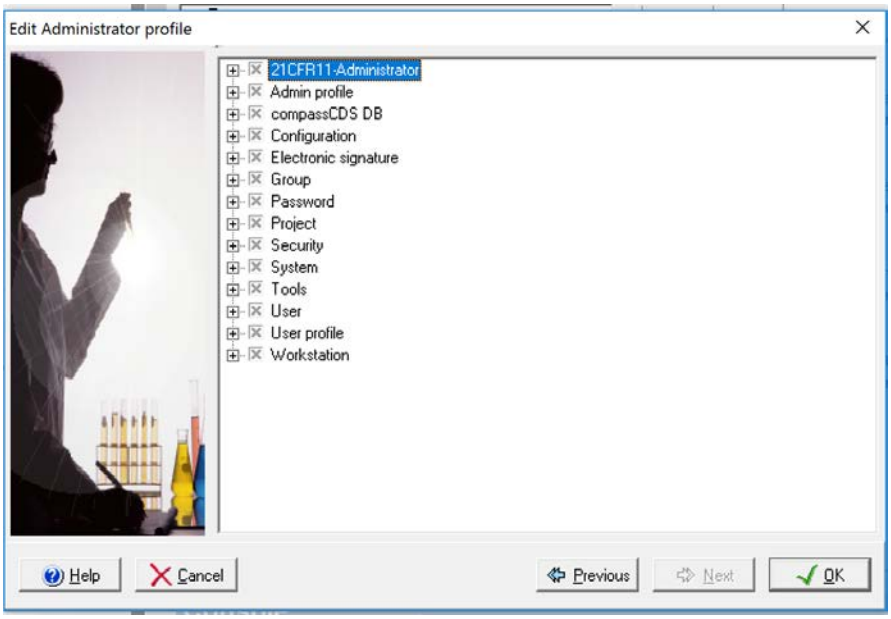
The Admin profiles properties wizard will appear:



Enter the Profile Name (40 characters maximum), and the description (255 characters maximum, optional.

The Use as default profile option can be checked in order to define this current Admin profile as default. Every time a new administrator is created, the default admiin profile will be assigned.

Clicking the *Next* button displays the second screen:



This screen defines the privileges allowed for this Admin profile, a privilege corresponds to an option within the CompassCDS Configuration Manager. Privileges are displayed grouped by sections and sub sections. To add/remove/modify privileges, an administrator selects each section from the list, then checks the box in front of the function to either allow it or unchecks the box to forbid it. If a function is unchecked, it will not be accessible to administrators with this admin profile in the CompassCDS Configuration Manager.

The following table lists the privileges available for use within Admin profiles:

Section	Sub sections	Action
Group	Create	Allow to create group
	Properties/ Modify name	Allow to modify group name
	Properties/ Modify description	Allow to modify group description
	Delete	Allow to delete group
	Overview	Allow to access the function that allows displaying only the connections of the item selected in the Item list.
Project	Create	Allow to create project
	Properties/ Modify name	Allow to modify project name
	Properties/ Modify description	Allow to modify project description
	Delete	Allow to delete project
	Overview	Allow to access the function that allows displaying only the connections of the item selected in the Item list
User	Create	Allow to create user
	Properties/ Modify name	Allow to modify user name
	Properties/ Modify user ID	Allow to modify user ID
	Properties/ Modify Initials	Allow to modify user initials
	Properties/ Modify description	Allow to modify user description
	Properties/ Modify e-mail address	Allow to modify the e-mail address
	Properties/ User account	Allow to change the user account
	Properties/ Log on all my projects	Allow to log on all my projects
	Properties/ Change password	Allow the administrator to change password (from CM)
	Allow the user to change his password from CDS application	Allow the user to access the change password option in CompassCDS
	Properties/ Modify allowed stations	Define the stations allowed for this user
	Properties/ Modify administrator rights and profile	Allow to give the administrator right to a user and to define the associated admin profile
	Properties/ Do not allow multiple logons	Forbid user to connect in several CompassCDS Chromatography Data sessions.
	Delete	Allow to delete user
	Overview	Allow to access the function that allows displaying only the connections of the item selected in the Item list.
User Profile	Create	Allow to create user profile
	Properties/ Modify name	Allow to modify user profile name
	Properties/ Modify description	Allow to modify profile description

Section	Sub sections	Action
	Properties/ Define profile by default	Allow to define user profile as default user profile
	Properties/ Modify privileges	Allow to access the privileges list of user profile and to modify it.
	Properties/ Modify token directory mask	Allow to modify the token mask
	Delete	Allow to delete user profile
Admin Profile	Create	Allow to create admin profile
	Properties/ Modify name	Allow to modify admin profile name
	Properties/ Modify description	Allow to modify admin profile description
	Properties/ Define profile by default	Allow to define admin profile as default admin profile
	Properties/ Modify privileges	Allow to access the privileges list of admin profile and to modify it
	Delete	Allow to delete profile
Station	Create	Allow to create station
	Properties/Modify name	Allow to modify station name
	Properties/Modify description	Allow to modify station description
	Properties/Define as acquisition server	Allow to define the station as acquisition server
	Properties/Lock	Allow to lock or unlock the station
	Properties/Modify users allowed	Allow to modify users allowed to connect to the station
	Delete	Allow to delete station
System	Create	Allow to create system
	Properties/Modify name	Allow to modify system name
	Properties/Modify description	Allow to modify system description
	Properties/Modify laboratory name	Allow to modify laboratory name
	Properties/Modify acquisition server	Allow to modify associated acquisition server
	Properties/Modify sequence server	Allow to modify associated sequence server
	Properties/Lock	Allow to lock /unlock the system
	Properties/Modify driver selection	Allow to modify the drivers selection
	Properties/Modify injector logical name	Allow to modify the injectors logical name
	Properties/Modify detector name and unit	Allow to modify the detector unit and conversion factor
	Properties/Configure system	Allow to configure system
	Start or stop system	Allow to start or stop system from CM
	Delete	Allow to delete system
Security	Lock user account after successive failed attempts	Allow to lock user account after successive failed attempts
	Lock administrator account after successive failed attempts	Allow to lock administrator account after successive failed attempts
	Lock session after a period of inactivity	Allow to lock the session after a defined period of inactivity
	Lock on user decision	Allow to lock the station on user decision
	Hide user at logon	Allow to hide the user identification at logon

Section	Sub sections	Action
	Password	Minimum password length
	Maximum user password age	Access the maximum password age parameter of user password
	Maximum administrator password age	Access the maximum password age parameter of administrator password
	History	Access the history parameters
Tools	License manager/ Add	Allow to add license
	Print the database	Allow to print the database
	Available devices	Access the available devices menu
Configuration	Organization/ Current organization	Allow to modify association between items in the organization configuration screen
	Organization/ Change paths	Allow to modify paths
	Organization/ Change systems	Allow to modify the systems association
	Parameters/ Calibration curve orientation	Allow to modify the calibration curve orientation (response versus concentration or concentration versus response)
	Parameters/ Message of the day	Allow to modify the message of the day
Electronic signature	Change electronic signature parameters	Allow to modify electronic signature parameters
21CFR11-administrator	Parameters to list in the audit trail	Allow to define the items and events to list in the audit trail
	View audit trail	Allow to display the current audit trail
	Create archive	Allow to create archive of the current audit trail
	Identification for archive creation	Forces the admin to enter User ID and password when archiving the CM audit trail
	View archive	Allow to view an archived audit trail
	Create archive and clear current audit trail	Allow to create archive of the current audit trail and to clear it
	Can read reasons & comments	Allow to read reasons & comments in audit trail
	Mandatory reason for change	Force user to enter a reason when he changes some parameters in CM
	Mandatory comments for change	Force user to enter comments when he changes some parameters in CM
	Modify reasons for Configuration Manager change list	Allow administrator to modify the list of reasons for changes in CM
	Modify reasons for Chromatography Data System change list	Allow administrator to modify the list of reasons for chromatogram changes in CompassCDS
	Modify reasons for chromatogram lock list	Allow administrator to modify the list of reasons for chromatogram lock in CM

NOTE: To de-select all the privileges of a section or of a sub section in a single step, uncheck the section or sub -section title.

If all the privileges of a section or sub-section are unchecked, the section or sub- section title can be checked to select all the associated privileges in a single step.

NOTE: To apply the changes made in the admin profile, a connected administrator to whom the modified admin profile has been assigned the current administrator who created the profile must log out of the Configuration Manager session and the new administrator must then log in.

Enter the changes made by clicking the *OK* button.

Editing a Admin Profile

To change any information concerning a particular admin profile, an administrator double clicks on the admin profile name, or selects the *Edit* option in the admin profile popup menu. This will access the properties screen, and user can make changes as needed.

The User Profile

The User profile represents the rights (permissions or privileges) assigned to a user when /user logs in to a CompassCDS session.

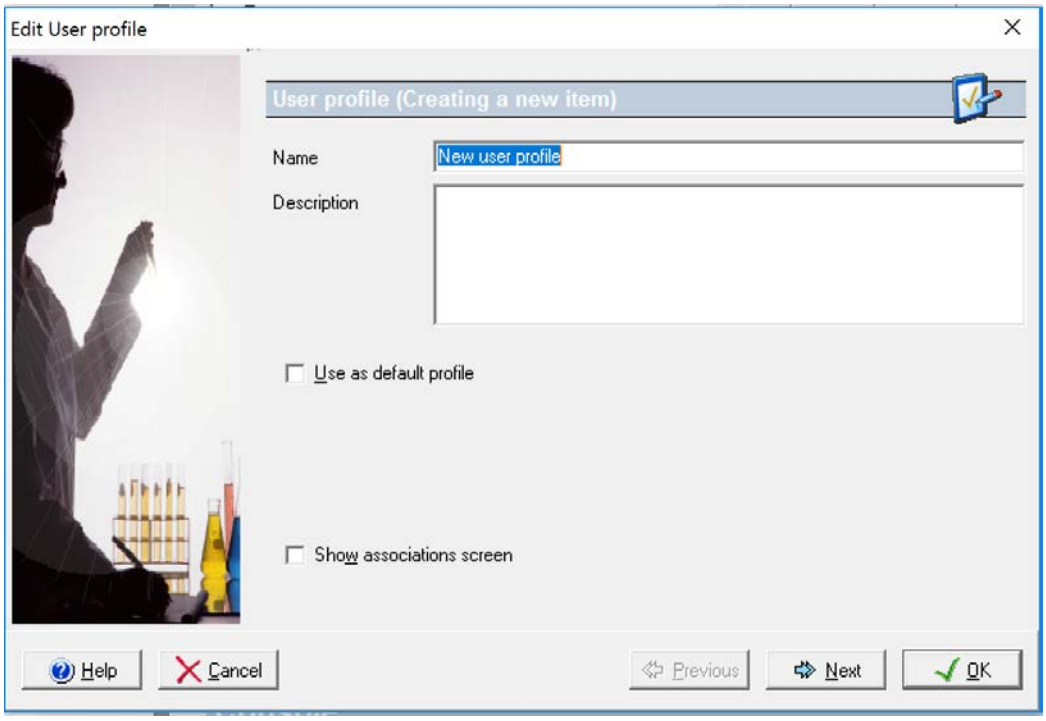
To display the User profile parameters, the

icon in the organization browser is selected.

Creating a New User Profile

Right click in the *User profiles* panel, and select the *NEW* option in the popup menu, or select the *USER PROFILES / NEW* menu.

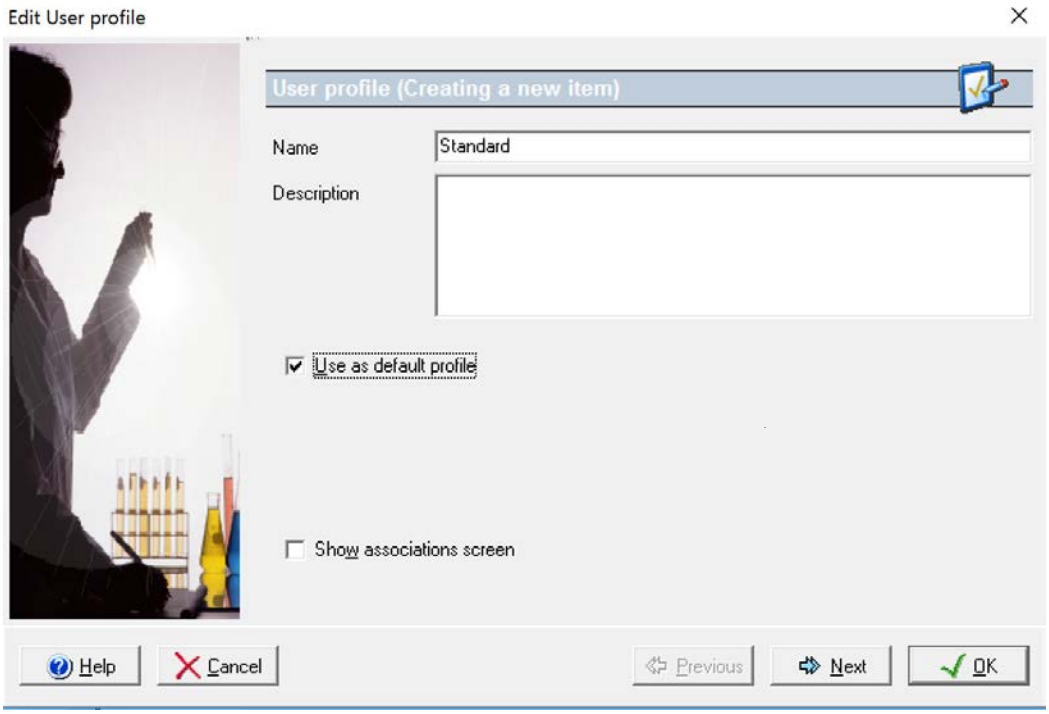
The User profiles properties wizard will appear:



Enter the Profile Name (40 characters maximum), and the description (255 characters maximum, optional).

To define this current User profile as default, the Use as default profile option can be checked. Every time a new user is associated with a group/project, the user is then automatically assigned the default user profile.

Clicking the *Next* button advances to the second screen:



This screen defines the privileges associated with a particular User profile. A privilege corresponds to an option within CompassCDS. Privileges are displayed grouped by section and sub-sections. To enable a privilege and make it available within CompassCDS, it is selected from the list and the checkbox that precedes that function is checked. To disallow the privilege, the box is unchecked. If a function is unchecked, it will not be accessible to users with this user profile in CompassCDS.

The following table lists the privileges available for use within User profiles:

Section	Sub sections	Action
File	Close all	Closing all opened files
	Save all	Saving all opened files
	Quit	Closing the CompassCDS Chromatography Data System session
	Preferences	Access the preferences menu (keep in memory system channel colors, show console, etc.)
Display	Display data tab	Display the Data tab
	Display systems tab	Display the Systems tab
	Display calibration tab	Display the Calibration tab
	Display toolbars	Display toolbars
	Display Audit Trail	Display the Audit Trail
	Display suitability log	Display suitability log

Section	Sub sections	Action
Chromatogram	Open chromatogram	Access the function: open chromatogram
	Close chromatogram	Access the function: close chromatogram
	Edit chromatogram properties	Access the function: chromatogram properties
	Save chromatogram	Access the function: save chromatogram
	Save Chromatogram Method	Allow the user to overwrite the method associated to the chromatogram with the current chromatogram one
	Lock/ Lock chromatogram	Allow the user to lock chromatogram
	Lock/ Unlock chromatogram	Allow the user to unlock chromatogram
	Lock/Mandatory reason for chromatogram lock/unlock	Force user to enter a reason when locking or unlocking a chromatogram.
	Lock/Mandatory comment for chromatogram lock/unlock	Force user to enter comments when locking or unlocking a chromatogram.
	Chromatogram display/ Display peak properties	Display the peak properties
	Chromatogram display/ Show peak markers	Display the peak markers
	Chromatogram display/ Show peak name	Display the peak name
	Chromatogram display/ Show baseline	Display baseline
	Chromatogram display/ Show event markers	Display event markers
	Chromatogram display/ Show event name	Show event name
	Chromatogram display/ Show peak identification window	Display peak identification window
Method	New method	Access the function: new method
	New method from template	Access the function: new method from template
	Open method	Access the function: open method
	Close method	Access the function: close method
	Save method	Access the function: save method
	Save method as	Access the function: save method as
	Save method as template	Access the function: save method as template
	Edit variables	Editing of the variables (method menu)
	Edit control parameters	Editing of the control parameters
	Edit acquisition parameters	Editing of the acquisition parameters
	Edit preprocessing parameters	Editing of the pre-processing parameters
	Edit integration event parameters	Editing of the integration events

Section	Sub sections	Action
	Edit peak identification parameters	Editing of the peak identification table
	Edit group identification parameters	Editing of the group identification table
	Calibration/ Edit calibration parameters	Editing of the calibration parameters
	Edit format parameters	Editing of the formats (peaks, groups and chromatograms)
	Edit peak report format	Editing of the peak report
	Edit group report format	Editing of the group format
	Edit chromatogram format	Editing of the chromatogram format
	Edit peak annotation	Editing of the peak annotation (icon and display menu / annotation)
	Edit event annotation	Editing of the annotation events (icon and display menu / annotation)
	Edit suitability test parameters	Editing of the suitability tests parameters
	Edit export parameters	Editing of the export parameters
	Edit post processing parameters	Editing of the post processing parameters
	Edit report style parameters	Editing of the printing report parameters
	Edit summary report parameters	Editing of the summary report list associated to the method
	Column Ageing	Activation of the Column Ageing function
	Retention index	Activation of retention index calculation function (associated to edit peak identification parameters)
	Retention index for olfactometry	Activation of retention index calculation function for olfactometry (associated to edit peak identification parameters and retention index)
	Ability to create variables	Allows the user to create variables
	Ability to lock variable	Allows the user to lock user input or user formula variables
	Ability to delete variables	Allows the user to delete variables
	Overwrite variable repository	Allow the user to overwrite the variable repository with the current one.
Reporting	New report style	Access the function: new report style
	Open report style	Access the function: open report style
	Print	Access the print function
	Print preview	Access the print preview function
Baseline Monitoring	Start monitoring baseline (etc.)	Access the monitoring baseline function (initial conditions).
Acquisitions/ systems properties	Stop all acquisitions	Access the stop button on all acquisitions started
	Use token directory for data path	Create automatic project subdirectory to store chromatogram files

Section	Sub sections	Action
	Can modify all acquisition run lengths	Allow to modify the acquisition length of all acquisitions
	Can modify acquisition run length of acquisitions started by the connected user	Allow to modify the acquisition length of acquisitions started by the connected user
	Allow to discard buffered files	Permission to discard acquisitions points stored in the MIB Interface Buffer
	Allow to start and stop systems	Allow to start and stop systems from CompassCDS. Can be used in case of communication problem with the chromatographic system
	Mandatory reason for start and stop systems	Force user to enter a reason when he starts or stops a system
	Mandatory comment for start and stop systems	Force user to enter comments when he starts or stops a system
	Allow to run instrument maintenance software	Allow the user to access the instrument maintenance software.
Quick start	Start Quick start	Access to the Quick start function
Sequence	New sequence	Access the new sequence function
	Do not overwrite sequence	To prevent user from overwriting a sequence
	Enable automatic save	To create a sequence which name is sequence name time stamp each time a sequence is run. This option has to be activated if token name have been defined in the chromatogram name (acquisition parameter), and the user wants to create a REPL from the sequence, or sign a batch of chromatograms coming from this sequence.
	Open sequence	Access the open sequence function
	Start sequence	Access the start button in the sequence
	Stop sequence	Access the stop button in the sequence
	Pause sequence	Access the pause button in the sequence
	Save sequence	Access the save sequence function
	Save as sequence	Access the save as sequence function
	Close sequence	Access the close sequence button
	Use remote sequence	Provides access to the remote sequence option
Processing	Integrate	Access the integrate function (icon, processing menu)
	Reprocessing single / Integration	Access the integrate function of the reprocessing single screen
Reprocessing list	New reprocessing list	Access the new reprocessing list-function
	Open reprocessing list	Access the open reprocessing list function
	Start reprocessing list	Access the start button in the reprocessing list
	Save reprocessing list	Access the save reprocessing list function
	Save as reprocessing list	Access the save as reprocessing list function

Section	Sub sections	Action
	Do not overwrite reprocessing list	Prevent a user from overwriting the reprocessing list
	Stop reprocessing list	Access the stop button in the reprocessing list
	Close reprocessing list	Access the close reprocessing list button
Manual Integration	Select mode	Access the select peak icon
	Move marker mode	Access the move marker icon
	Add peak mode	Access the add peak icon
	Delete current peak	Access the delete peak icon
	Undo last action	Access the undo last action icon
	Split peak mode	Access the split peak icon
Calibration curve	Open calibration curve	Access the open calibration curve function
	Do not overwrite calibration curve	Prevent a user from overwriting the calibration curve
	Close calibration curve	Access the close calibration curve function
	Save calibration curve	Access the save calibration curve function
	Open calibration curve	Access the open calibration curve function
	Use M and D factors for curve building	To allow the user to build calibration curve using M and D factors for standards (if the profile is not activated those factors are not used, even if they are assigned values). M and D are equally used for the quantification of standard samples
Results	Manual operations	Access the manual operations list applied to a chromatogram
	Peak results	Access the peak results table
	Group results	Access the group results table
Summary report	New summary report	Access the new summary report function
	Open summary report	Access the open summary report function
	Save summary as	Access the save summary as function
21CFR11-user	Chromatogram management/ Do not overwrite chromatogram	Prevent a user from overwriting chromatograms when running a Quick start or a sequence
	Chromatogram management/ Print as PDF	Access the PDF generation option
	Audit trail/ Archive method	Archive successive versions of methods
	Audit trail/ Archive chromatogram	Archive successive versions of chromatograms
	Audit trail/ Archive calibration curve	Archive successive versions of calibration curves
	Audit Trail/ Archive sequence	Archive successive versions of sequences
	Audit Trail/ Archive reprocessing list	Archive successive versions of reprocessing lists
	Audit trail/ Mandatory reason for change	Users chooses a reason from a list to justify the change
	Audit trail/ Mandatory comment for change	To force the user to enter a comment to justify the change made
	Audit trail/ Do not clear audit trail	To prevent a user from clearing the audit trail

Section	Sub sections	Action
	Audit trail/ Do not get archive	To prevent a user from accessing the get archives button and allowing user to update an archive
	Audit trail/ Ability to see reason and comments	To access the option that displays the reason and comments entered by user when he saved the file
	Electronic signature/ Sign off chromatograms	Allow access to the Chromatogram Sign off function
	Electronic signature/Review chromatogram signatures	Allow access to the Chromatogram Signature review function
	Electronic signature/ As representative of sign off user for chromatograms	Allow user to sign only this chromatogram
	Electronic signature/Allow batch sign at once	Allow the user to sign in a single step a selection of chromatograms.
Session	New login	Access the new login function. ALL the parameters of the database must be considered (profiles, system rights, etc.)
Help	Help	Access the on-line help
	About	Access the about screen

If the *Acquisitions / systems properties / use token directory for data path* privilege has been selected, the *Next* button becomes available. Clicking on it will display the following screen:

A token is a tool that enables a user to automatically create a directory in which the acquisitions (quick start or sequence) the user performs will be stored. This directory is always a sub-directory of the project directory.

A token is defined by variable(s) and/or text, which must be defined in the previous screen.

To define variables in the token mask, an administrator clicks the

button, and then double clicks on the variable name to be added. Several variables can be defined in the same token mask. The available variables are:

$Day1: Day with one digit minimum from 1 to 31.

$Day2: Day with two digits minimum from 01 to 31.

$Daylong: Day from Monday, Tuesday to Sunday.

$Dayshort: Day with three characters from Mon, Tue to Sun.

$Group: Group in which the user has logon.

$Initials: Initials of the operator as defined in the Users/Edit wizard.

$Logon: Current logon name.

$Month1: Month with one digit minimum from 1 to 12.

$Month2: Month with two digits minimum from 01 to 12.

$Project: Project in which the user has logon.

$System: Name of the system on which the acquisition was performed.

$Week: Week of the year from 1 to 52.

$Year2: Year with two digits minimum from 00 to 99.

$Year4: Year with four digits minimum from 1999 to 9999.

$Laboratory: Name of the laboratory that owns the system that performs the acquisition.

The variable names can be typed by the administrator. In this case, it is important to remember to precede the variable name by '$'. Characters other than listed variables will be created as these are entered. As a consequence, it is important to not enter any point or slash in this window.

For example, if a token QC_$Initial_$Day2_$Month2 is entered, the chromatograms are saved in a directory named QC_JD_05_12, if the user John Doe starts a sequence on the fifth of December.

It is also possible to create different levels of token by defining a '\' between variables. For example Year4\Month2\Day2, creates a directory for the year, then a sub directory for the month, and then a sub directory for the day.

Enter the changes made by clicking the *OK* button.

Editing a User Profile

To change any information concerning a particular user profile, just double click on this user profile name, or select the *Edit* option in the user profile popup menu to access the properties screen, and make the changes as needed.

The Stations / Systems Items

The CompassCDS Configuration Manager allows the administrator to manage all the stations and systems connected to a CompassCDS network.

The Station

A station represents the computer on which CompassCDS is installed.

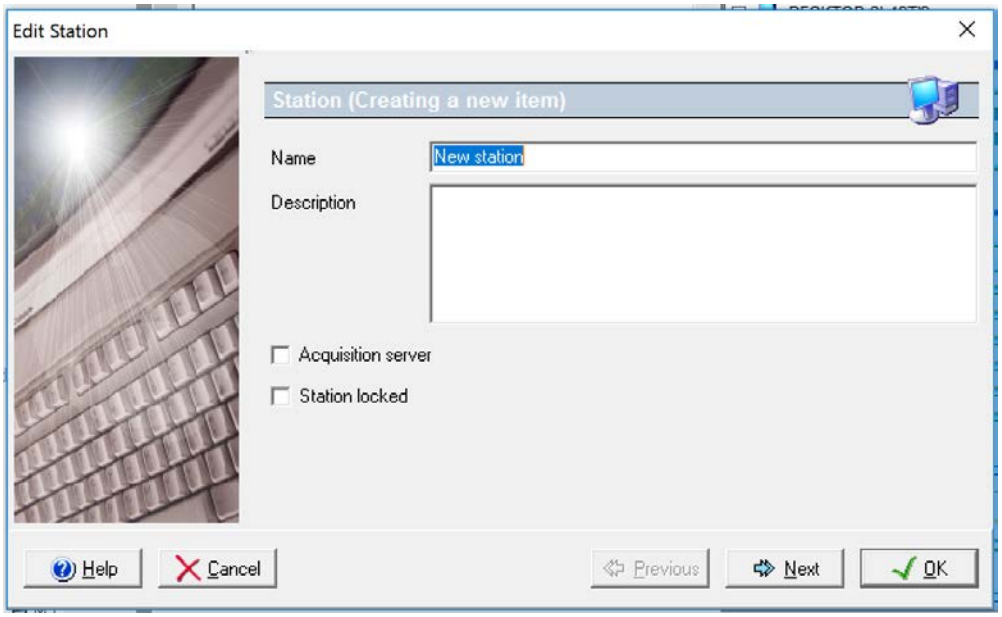
To display the Station parameters, select the

icon in the Stations / Systems browser.

Editing a Station

To change any information concerning the station, just double click on this station name, or select the *Edit* option in the station popup menu to access the properties screen, and make the changes as needed.

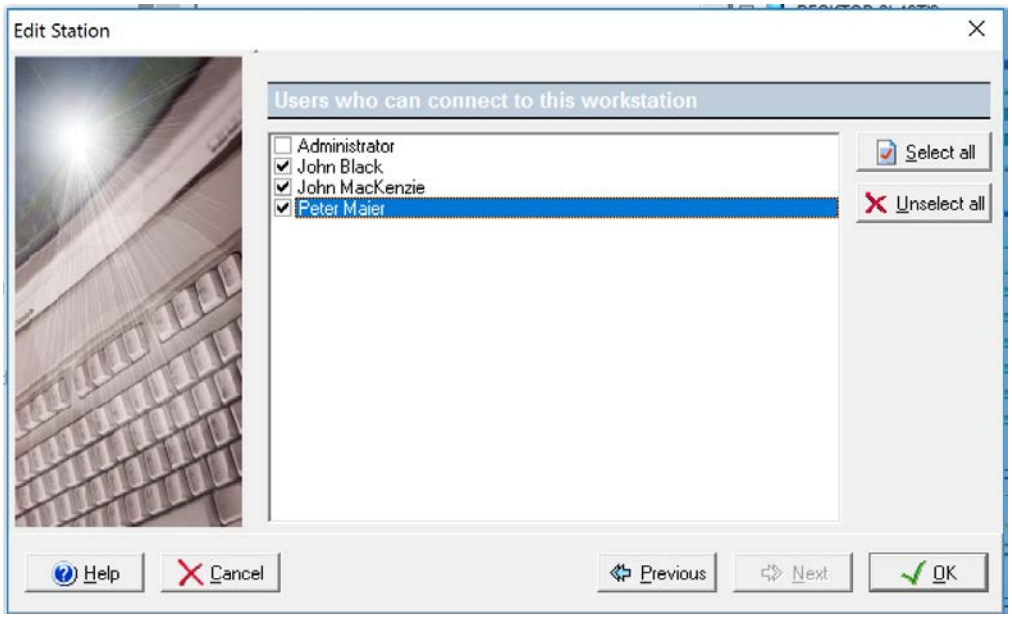
The Station properties wizard appears:



Fill in the following information:

- Name: Name of the station (40 characters maximum),
- Description: Description of the station (255 characters maximum), this field is optional.
- Station locked: Allows the administrator to temporarily lock the current station. No one will be able to log on to CompassCDS or on to the CompassCDS Configuration Manager from this station while it is locked. When a station is locked, it is displayed with the symbol in the station list and in the stations / systems screen.
- Acquisition server: This is a very important field that indicates that the station is designated as an acquisition/control server of the systems. This option MUST be checked.

Press the *Next* button to advance to the second screen:



In this screen, you have to define the list of users that will be authorized to start a CompassCDS session on this station.

The System

A system represents a chromatographic system, composed of different modules (autosampler, detector, etc.). Systems are running as services. Each time a system is running, the corresponding service is started.

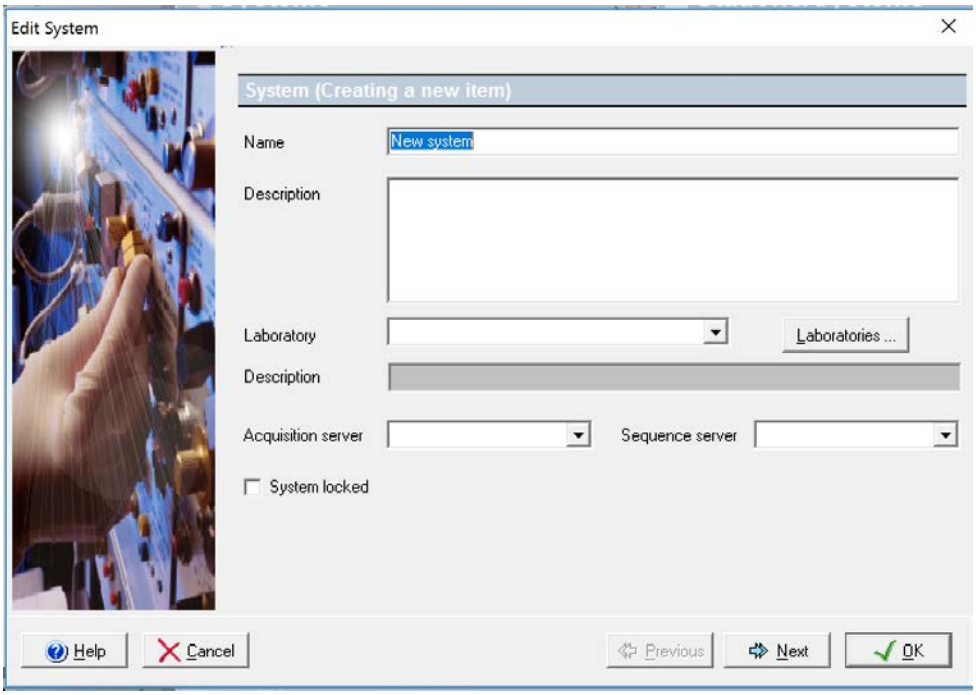
To display the System parameters, select the

icon in the Stations / Systems browser.

Creating a New System

Right-click in the *Systems* panel, and select the *NEW* option in the popup menu, or select the *SYSTEMS / NEW* menu.

The System properties wizard appears:



Fill in the following information:

- Name: Name of the system (40 characters maximum). The characters that are authorized are: alphanumeric characters, spaces, minus signs, plus signs and underscores.
- Description: A description of the system (255 characters maximum), this field is optional.
- Laboratory: The name of the laboratory that owns the system (40 characters maximum), this field is optional.
- Acquisition server: To define the station that manages the system.
- Sequence server: To define the station that manages the acquisitions performed on this system.
- System locked: Allows the administrator to temporarily lock the system, that will not be accessible from any station, neither Acquisition nor Control will be possible. This is useful for the routine maintenance of an instrument. When a system is locked, it is displayed with the symbol in the station list and in the stations / systems screen.

To define, modify or delete a laboratory, press the

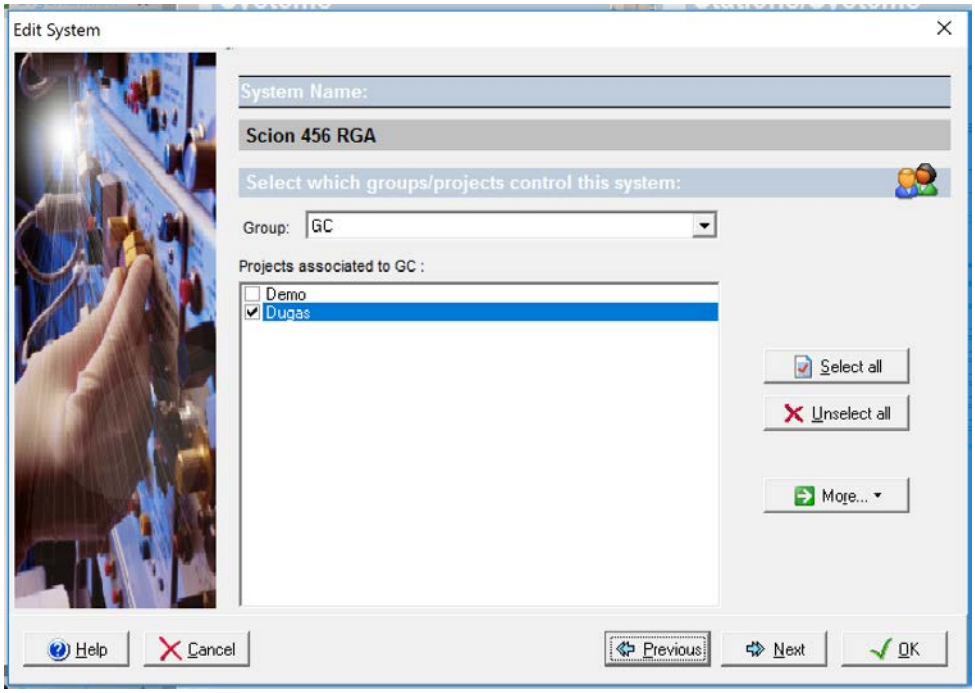
icon. The following screen will be displayed:

Press the *New* button to create a new laboratory. A laboratory is defined by a name (40 characters maximum) and optionally a description (255 characters maximum).

Press the *Delete* button to delete a selected laboratory.

Press the *Properties* button to modify a selected laboratory.

Press the *Next* button to advance to the second screen:

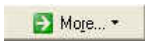


It is possible in this screen to select the group(s) and then, the project(s) to which the system will be directly associated.

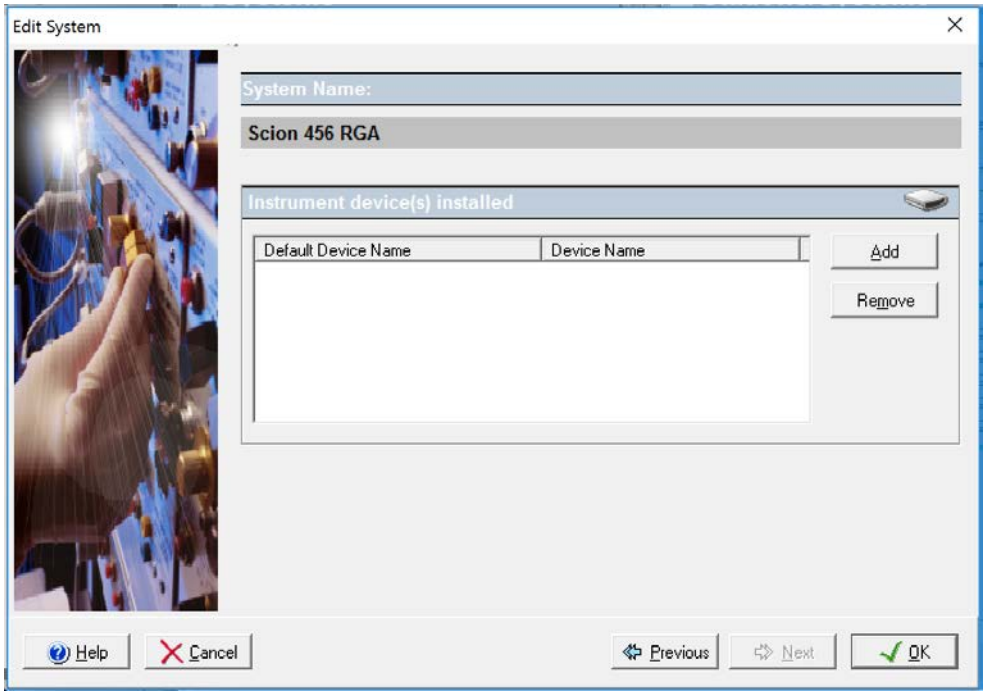
To assign the system in a single step to all the projects of a group, press the button.

To remove the system in a single step from all the projects of a group, press the button.

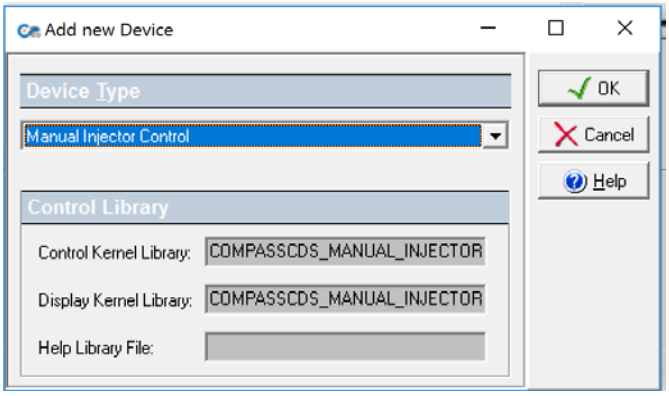
To associate the system to a selected project in all groups, select first the desired project and press the button in order to select the *Associate to the selected project in all groups'* option. Remove the system from the select project in all groups using the *Remove from the selected project in all groups'* option.

To associate the system to all defined groups/projects associations, press the  button and select the *Associate to all groups/projects* option. Remove the system from all defined groups/projects to the *Remove from groups/projects* option.

Press the *Next* button to advance to the third screen:



To select a module, press the *Add* button, the following screen is displayed:



Select in the *Device type* list the module of interest, and then click on *OK*. The corresponding module is then listed in the list of instrument devices involved in the system.

NOTE: Each system is required to have an injector configured in the system. If an autosampler is not configured in the system, then the manual injector control device must be included in the system.

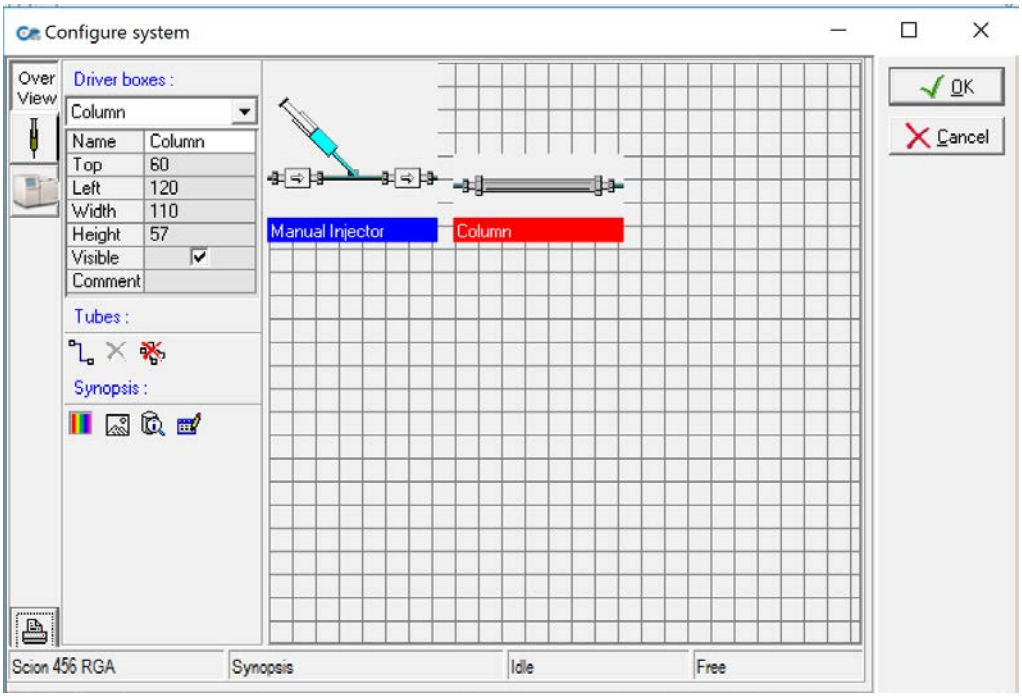
If the *Device Type* list is empty or does not contain the required instrument module device, you have to install the corresponding licenses via the set up or the OPTIONS / LICENSES menu. The OPTIONS/ DEVICES menu allows service people to install or update drivers with prerelease or beta drivers for testing.

Repeat this operation for each instrument module.

If you need to remove a module from the *Instrument device(s) installed list*, select its name and click on the *Remove* button.

Then click on *OK*.

A prompt appears to ask if the instrument device must be configured. If the response is Yes, the instrument device configuration screen appears.



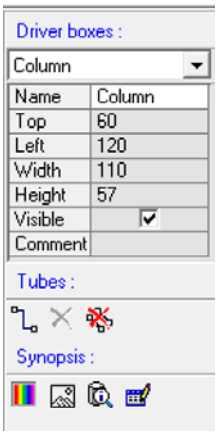
This screen displays several tabs corresponding to the installed instrument modules.

For each instrument module, define all the hardware parameters, such as the currently installed options found on this instrument (syringe volume, special detector, etc.), or the type of hardware connection to CompassCDS, etc. Please refer to the specific CompassCDS driver manual for information about the specific instrument parameters.

After having configured your system (injector type, detector type, etc.), you may define a ‘Synopsis’ (overview tab). The synopsis is a representation of the chromatographic system, that will be displayed in the acquisition view in CompassCDS, and that will display the instruction and the real value of the parameters (temperature, pressure, etc.).

Depending on the installed devices, specific pictures are displayed. The user has to link these devices one to the other via connection tubes, to create a schematic of his system.

To create the synopsis, the user can place the devices at the desired position using the mouse, or define the position in the table:



Then the objects can be joined using the tubes by first selecting the two parts to link, then selecting the icon, a tube is displayed.

To delete a tube, select it then click on the icon.

To delete all the tubes, select the icon.

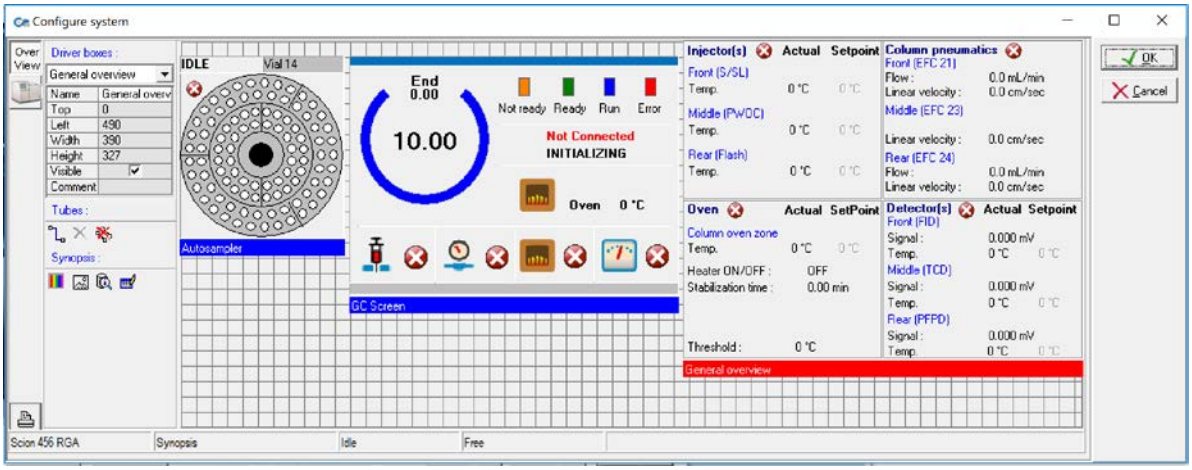
To change the background color, select the icon.

To display a transparent background, select the icon.

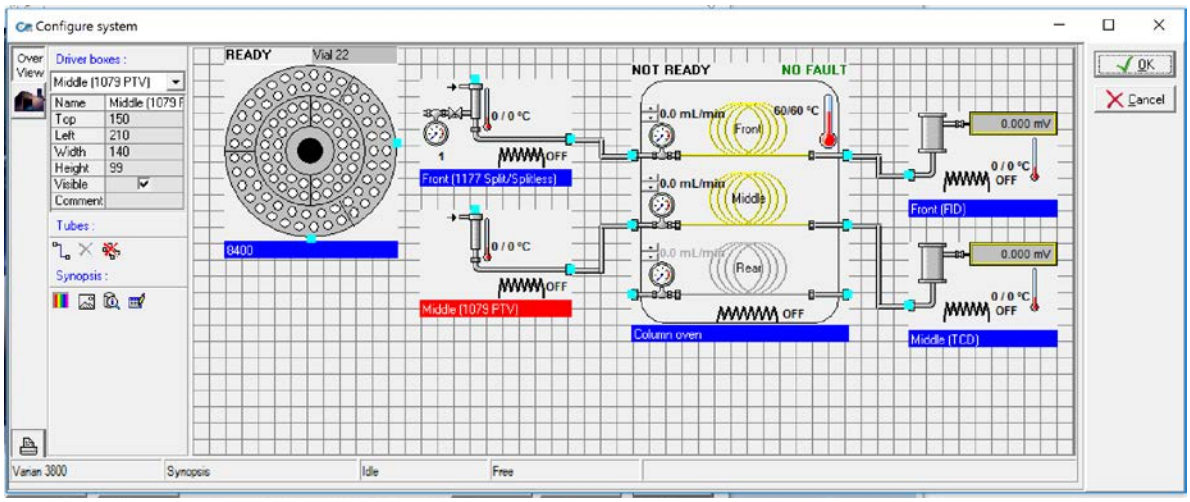
To display the last modifications select the icon. No archives are created, so only actions performed before accepting the changes by clicking *OK* are listed.

To change the grid color, select the icon.

The following picture represents the synopsis of the Scion 456 GC.



The synopsis system will be displayed in CompassCDS System tab, with some status information (temperature, flow, depending on the installed drivers). For the Varian 3800 GC system, the synopsis is displayed as follows; the set and actual values are displayed.

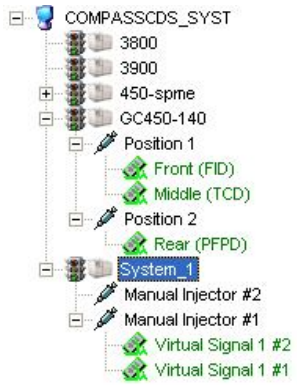


Changing Injector/Detector Association

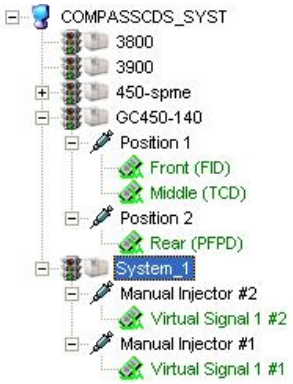
Any system can have multiple injection devices and multiple detectors. This is typically the case on some GCs that have dual injectors and up to 4 detectors.

In the CompassCDS Configuration Manager, in some cases of multiple injector/detector on the same system, the association may have to be defined by the user. The system is not always able to know how the devices are linked to a system.

Before doing any association, a system looks like this:



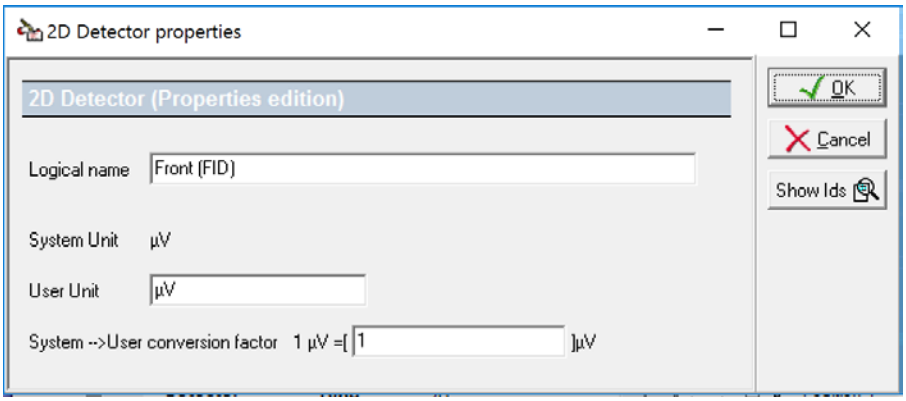
For example, to associate the detector to the system, highlight the detector and drag and drop to the injector item. Now, the system looks like this:



NOTE: Injector does not necessarily mean an autosampler or an auto injector. It can represent any injection device, including a manual injector.

Changing Detector Properties

To change the logical name of the detector and the signal units, select the detector in the *Stations/Systems* screen, and press the right mouse button, then select *Properties.*

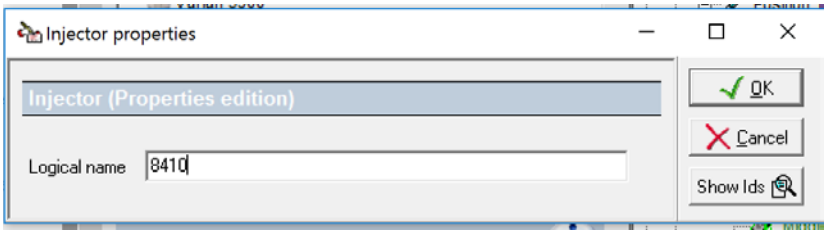


The system unit is µV by default, but it can be modified to display another unit. To change the unit, enter the User unit then the conversion factor in the corresponding box. The chromatograms drawn in CompassCDS as well as the height results will use the selected Unit.

Press the *Show Ids* button to display the triplet identifier of the detector. This option is useful for service people.

Changing Injector Properties

To change the logical name of the injector, select the injector in the *Stations/Systems* screen and press the right mouse button, then select *Properties*.



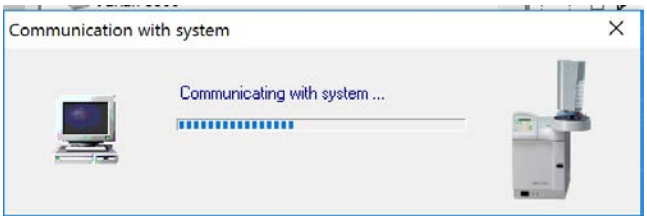
Press the *Show Ids* button to display the triplet identifier of the injector. This option is useful for service representatives.

Stopping or Starting a System

It is possible to *Stop* or *Start* the system by running CompassCDS Configuration Manager. This function is useful when changing the hardware configuration of the system by adding a new detector or device, since it is done without causing an interruption within the entire lab.

Select the system in the *Stations/Systems* screen, and press the right mouse button. A menu appears with two options: *Stop* and *Start*.

By selecting one of these options, the CompassCDS Configuration Manager will try to contact the selected system and perform the action:



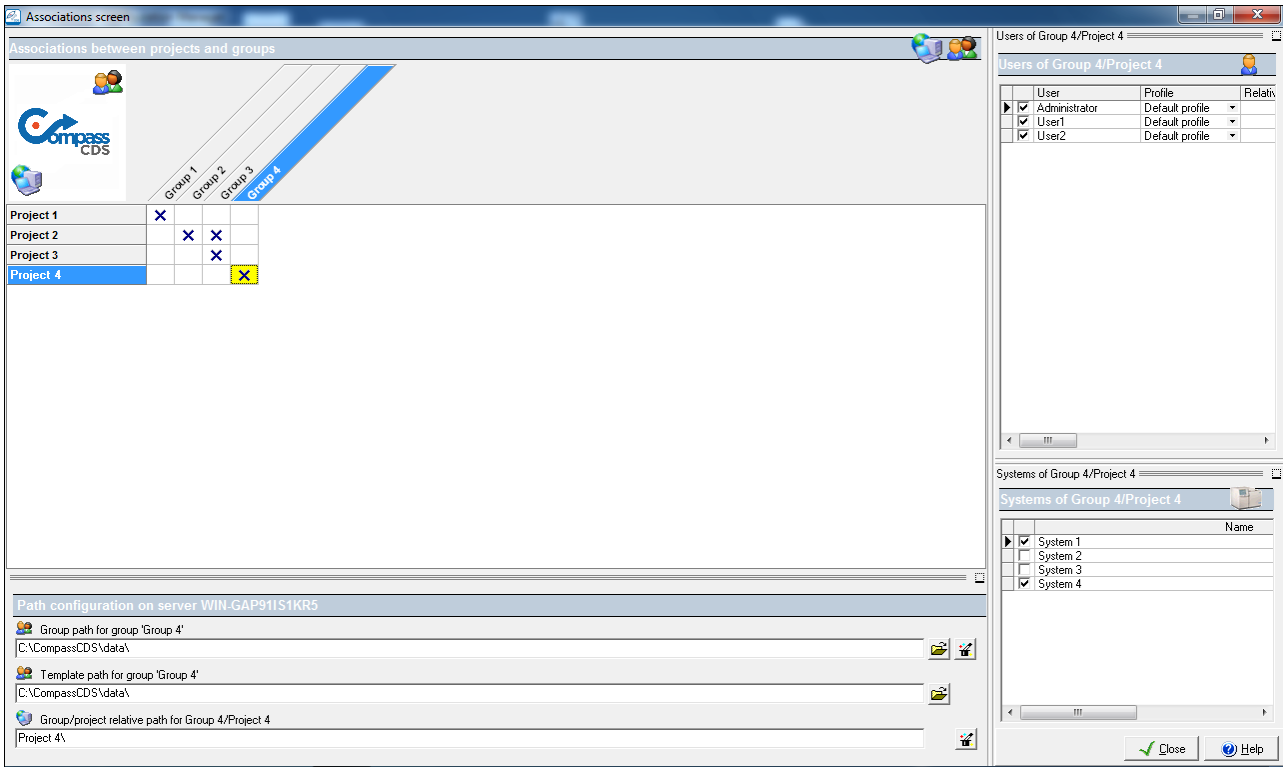
Editing a System

To change any information concerning a particular system, just double click on this system name, or select the *Edit* option in the station popup menu to access the properties screen, and make the changes as needed.

Organization Configuration (Items Associations)

Once the items are defined, you can define the way the items are linked to each of the others: group/projects – project/users- project/systems- user/user profile, and defined the associated paths.

Select the *CONFIGURATION / ASSOCIATIONS* menu, the *Organize* screen is displayed:



NOTE: You can access this screen from the item properties screen, by checking the *Show Associations Wizard* option or directly from the Organization tab.

The *Associations* screen allows the administrator to associate items or to edit defined association.

Association Creation

Association of a group to project(s):

Select one or several cells at the intersection of the groups and project lines (it is possible to use the CRTL and SHIFT keys to select several cells or to select in a single step the whole column by just clicking on the project or on the group name). These cells are displayed in yellow once selected. Both *group path* and *template path* are activated, allowing the administrator to define the paths.

The default group and template paths are: C:\COMPASSCDS\DATA, but these paths are modifiable. To automatically add the name of the group to the pre-defined path, click on the icon.

To associate project(s) to group(s), check the selected cells or use the *Associate* option in the popup menu. To associate projects to all the defined groups, select all the cells of the popup menu and associate them.

To remove one or several projects from a group, first select all the corresponding cells and uncheck them or use the *Remove* option present in the popup menu.

To remove the projects from all the defined groups, select all the cells and select then the *Remove* option.

Association of user(s) and system(s) to group/project(s):

Select a project associated to a group, the *Relative project path, the Users* list and the *Systems* list are activated. The project path is compulsorily a sub directory of the group path, so the relative path and not the complete path have to be defined. To add automatically the name of the project in the *Project relative path* field, click on the icon.

To associate one user or one system to the selected group/project, check the associated check box in the corresponding list or use the *Associate* option of the popup menu.

To associate several users or systems to one or several group/projects, select the cells corresponding to the group and to the desired project(s), and then associate the desired user(s) or system(s) (use the CTRL or SHIFT keys). The *Select all* option allows selecting all the users or systems and adding them to groups/projects.

To remove one or several users or systems from one or several group/projects, select the group and the desired project(s), then the desired user(s) or system(s) (use the CTRL or SHIFT keys) and then select the *Remove* option in the popup menu. To remove all the users or systems from groups/projects, first select the groups and projects and then all the users and systems and remove them.

NOTE: Systems are defined by group/project.

Association of a user profile to a group/project/user:

Select a user associated to a group/project, the user relative path and the profile scrolling list are activated. The user path is compulsorily a sub directory of the group path, so the relative path and not the complete path have to be defined. To automatically add the name of the user in the *User relative path* field, select the *Auto-path* option in the popup menu.

To associate a user profile to the selected group/project user, select it in the scrolling list.

To associate the same profile to several users belonging to the selected group/project, select the checked users in the list (use the CTRL or SHIFT keys), then select the *Apply same profile* option in the popup menu.

When associations are completed, click on the CLOSE button.

NOTE: A user profile is defined by group / project / user.

GENERAL NOTE: Changes made in this screen are available immediately.

GENERAL NOTE: The association between items can be done graphically from the main screen, by selecting the item in the corresponding *Item list* and drag and drop it on the desired position in the tree in the *Current organization* screen. A project can be associated to a group, a user can be associated to a group/project and a user profile can be associated to a group/project/user.

It is also possible to move an item from one position to another in the tree, by selecting it in the tree, drag and drop it in the desired position. The same association as those described just above are authorized.

In both cases: association or moving, remember to modify the paths in the Associations screen. By default, the group path is one of the new associated groups, and the relative project and user path are not modified.

Association Editing

It is possible to consult the defined association from the *Associations* screen accessible from the *CONFIGURATION / ASSOCIATIONS* menu or from the Organization tab.

- Editing of a group / project(s) association(s):
- Select the cell corresponding to a group/project association. Group, Template and Project relative paths are displayed in the corresponding fields.
- Editing of a group / project / user(s) + system(s) association(s):

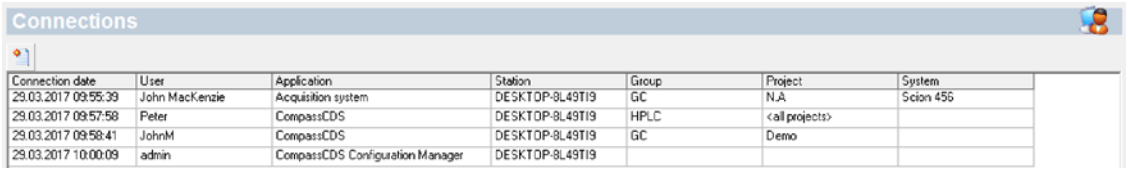
Select the group and the associated project (checked) in the *Groups* and *Projects* sections. The associated users and systems are displayed. Check in the *Users* and *Systems* lists.

Group, *Template*, *Project relative and Relative user* paths are displayed in the corresponding fields. The associated user profile is displayed in the corresponding scrolling list.

NOTE: It is possible to change any parameters in Editing mode. The same options as the ones described in the 'Association creation' section are available.

Connections

In the browser, select the Connections tab, the following screen is displayed:

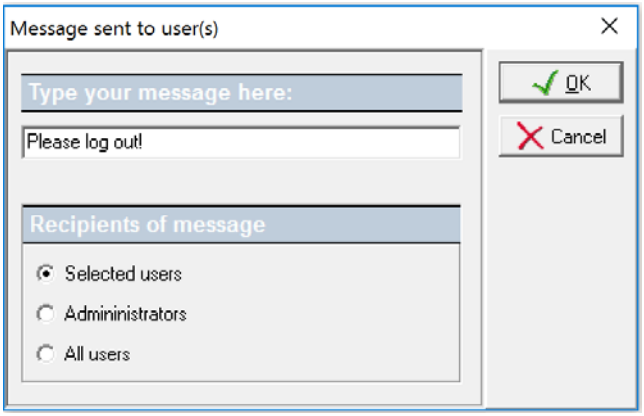


Connection date	User	Application	Station	Group	Project	System
29.03.2017 09:55:39	John MacKenzie	Acquisition system	DESKTOP-8L49TI9	GC	N.A	Scion 456
29.03.2017 09:57:58	Peter	CompassCDS	DESKTOP-8L49TI9	HPLC	<all projects>	
29.03.2017 09:58:41	JohnM	CompassCDS	DESKTOP-8L49TI9	GC	Demo	
29.03.2017 10:00:09	admin	CompassCDS Configuration Manager	DESKTOP-8L49TI9			

This screen displays the name of the connected administrator to CompassCDS Configuration Manager with the connection date and the station name, and the name of the connected users to CompassCDS with the connection date, the station name and the group and project user is connected in. It also displays the acquisitions that are running, on which station and system they are running and the name of the user that is connected in the group/project and that has started the acquisitions.

Select the *Send message* option in the popup menu or the icon to send one or several user(s) and/or administrator(s) a prompt, for example to advise them to close the application before a change in the configuration is done.

The following screen is displayed:



Type the message in the corresponding field, then select the users you want to send it to. Three options are proposed:

Selected users (selected by default): Send to selected users and administrators that are highlighted in the connections tab.

Administrators: Send to all connected administrators (the selection is not necessary in this case).

All users: Send to all connected users (the selection is not necessary in this case).

Tools

In the browser, select the Tools tab. This screen content depends on the installed plug-ins or communication tools. An icon is associated to each installed tool in the browser. Those options are also available from the *OPTIONS* menu.

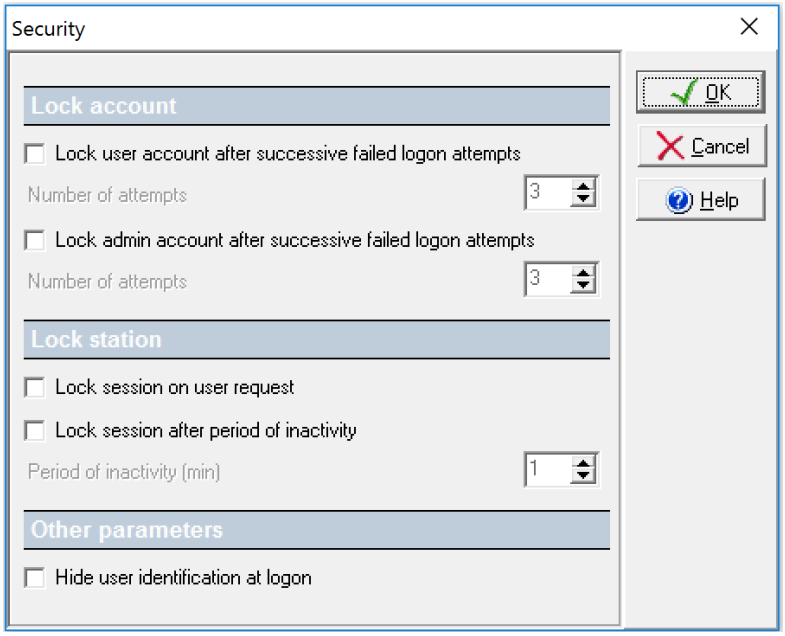
The more common tool is the BOOTP server. It is detailed in CompassCDS Installation Guide.

Configuration Parameters

This section describes the configuration parameters of the Configuration Manager: security options, password management, electronic signature configuration and general parameters. Those options are available from the *CONFIGURATION* menu.

Security

Select the *CONFIGURATION / SECURITY* menu. The following screen is displayed:



The following options are proposed:

Lock Account

Lock user account after successive failed logons attempts: If this option is selected, the user will be locked, if the specified number of failed logon attempts is reached when connecting to CompassCDS. When a user account is locked, it is displayed with a padlock both in the user list and in the Current organization screen. A user with a locked account cannot logon in CompassCDS.

In *Number of attempts* field, enter the number of failed logon attempts that will cause the account locking. The range is 1 to 99.

A locked user account can only be unlocked in the user properties in the CompassCDS Configuration Manager.

Lock admin account after successive failed logons attempts: If this option is selected, the administrator will be locked if the specified number of failed logon attempts is reached when connecting to a CompassCDS Configuration Manager. When an administrator account is locked, it is displayed with a padlock both in the user list and in the Current organization screen. An administrator with a locked account cannot logon, in CompassCDS, or in CompassCDS Configuration Manager.

In *Number of attempts* field, enter the number of failed logon attempts that will cause the account locking. The range is 1 to 99.

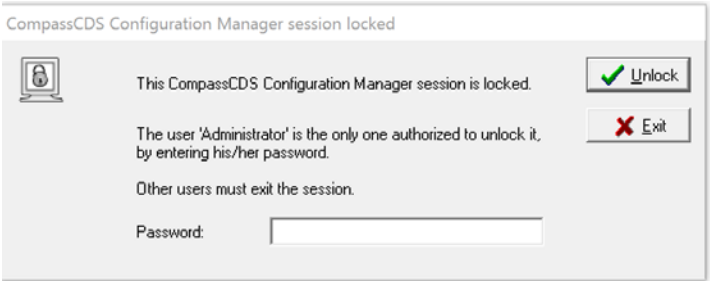
Lock Session

Two options are proposed to lock a station:

Lock session on user request*:* Allows the user connected in a CompassCDS session to lock its session when he wants, by selecting the corresponding option (not applicable to this version).

Lock session after period of inactivity: Allows locking automatically the CompassCDS software if the user does not perform any action for a certain period of time. By default, the session will never lock when CompassCDS is idle. Define the inactivity period in the corresponding time (from 1 to 99 min).

When CompassCDS or the CompassCDS Configuration Manager is opened but no action is performed during a time exceeding the specified time, the following window appears:


CompassCDS Configuration Manager session locked
This CompassCDS Configuration Manager session is locked.
Unlock
Exit
The user 'Administrator' is the only one authorized to unlock it, by entering his/her password.
Other users must exit the session.
Password:

It will be impossible to work in CompassCDS or in CompassCDS Configuration Manager any more until the connected user enters his password.

NOTE: If another user connects in this screen by entering its USER ID and password, the previous session will be closed; ALL CHANGES NOT SAVED, ARE LOST.

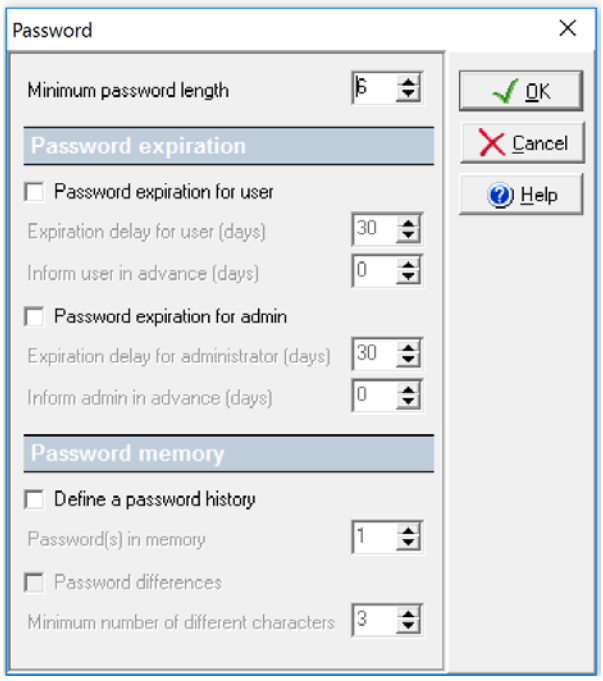
Other Parameters

One option is proposed:

Hide User identification at logon: Allows displaying the User ID in a non-readable way. Characters are replaced by ***.

Password

Select the *CONFIGURATION / PASSWORD* menu. The following screen is displayed:



The following options are proposed:

Minimum Password Length

This is the fewest number of characters that a password must contain. If this option is selected, the value can range from 0 (to not force a password to be defined) to 40 characters. The default value is 6.

Password Expiration

Password expiration for user: This option allows defining when user passwords have to be changed. Specify the limit time in the *Expiration delay for user* field (from1 to 365 days). After the expiration day, the user cannot log into CompassCDS without changing the password.

It is possible to ask for a password change a few days before the expiration date, by defining the corresponding time in the *Inform user in advance* field (from 0 day to defined Expiration delay). The user will then be able to change the password or to log into CompassCDS without changing it.

Password expiration for admin: This option allows defining when admin passwords have to be changed. Specify the limit time in the *Expiration delay for admin* field (from1 to 365 days). After the expiration day, the administrator cannot log into CompassCDS Configuration Manager without changing his password.

It is possible to ask for a password change a few days before the expiration date, by defining the corresponding time in the *Inform admin in advance* field (from 0 day to defined Expiration delay). The administrator will then be able to change its password or to log into the CompassCDS Configuration Manager without changing it.

NOTE: To change the password a user needs to enter the old password once, and enter the new one twice.

Password Memory

Define a password history: Allows realizing tests on the password, to force user to define a new password very different or totally different from his old ones. When this option is checked, the following options are available:

*Password in memory: A*llows defining the number of passwords the software will keep in memory (from 1 to 99).

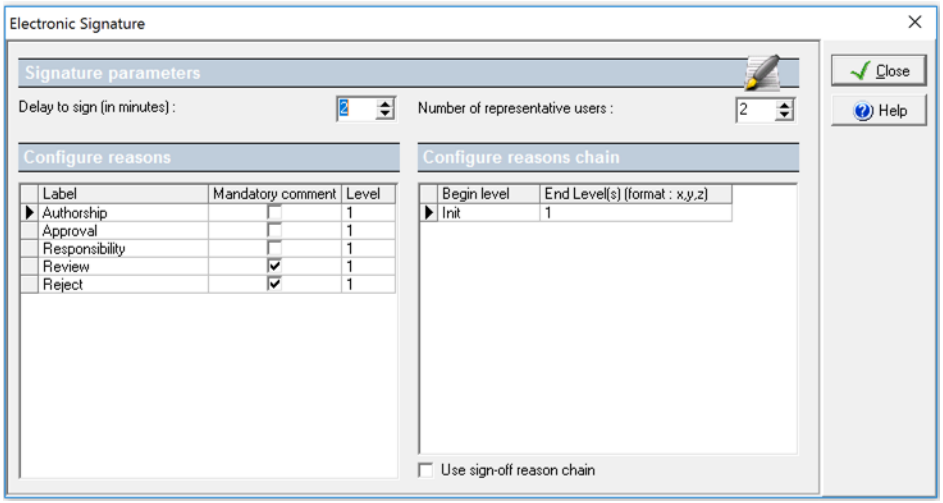
Password differences: If this option is checked, a test will be done to ensure the new password is different enough from the number of *password in memory* defined. An algorithm will estimate the number of differences (same characters, inversion of character position in the password) between all passwords kept in memory (from 1 to 40).

NOTE: In the case of empty password, the uniqueness test will always be accepted even if the character number is smaller than the ‘x characters’ condition.

NOTE: Each time a password is changed by an administrator (from the CompassCDS Configuration Manager); the user will be asked to change the password at first login.

Electronic Signature

Select the *CONFIGURATION / ELECTRONIC SIGNATURE* menu. The following screen is displayed:



The following options are proposed:

Delay to sign: Forces the user to sign the document before the delay ends. Delay can be set from 2 to 10 minutes. Once the delay has expired, the electronic signature screen closes and the document is not signed.

Number of representative users: This parameter sets the number of representative users who must sign the document instead of the user, when this option is selected in CompassCDS.

The number of representative users must be set to at least two.

Configure Reasons: In this table, the administrator can define a hierarchy for electronic signature reasons. He can configure the reasons, associate them a hierarchical level and associate a mandatory comment.

In the *Label* column, the administrator configures the reasons which will be available to the user when signing the chromatogram. By default, five reasons are defined and cannot be deleted: Authorship, approval, responsibility, review and reject. The administrator can add a maximum of 15 reasons. To add a reason select the *Add reason* in the popup menu associated to the table, and to remove selected reasons, select them and activate the *Remove selected reason(s)* option from the popup menu.

In the *Mandatory comment* column, the administrator can choose either to force the user to enter a comment when signing the chromatogram, or not.

In the *Level* column, the administrator specifies the reason level associated to each reason. This parameter will be used in the *Configure reasons chain* table.

Use sign-off reason chain: If this option is checked, a reason chain must be set in the Configure reason chain table. If this option is not checked, no sign-off reason chain is created. When the user signs the chromatogram, he can sign with all the reasons which are configured in the *Configure reasons* table.

Configure reasons chain: This option allows the user to set a hierarchy for electronic signature reasons. In fact, a chain of reasons can be created depending on the level defined in the *Configure reasons* table.

The administrator must define a *Begin level* and one or several *End level* for each step to link the reasons. He can define an unlimited number of links, modify the last defined step and remove the last defined step by selecting respectively the *Add step*, *Modify end level(s) of last step* or the *Remove last step* option in the popup menu.

Rules to complete the *Configure reason chain* table:

First, an initial level must be defined in the *Init* line, by activating the *Modify end level(s) of last step* option in the table popup menu. When the first user will sign a chromatogram in a CompassCDS session, he will be forced to select a reason which is assigned to the level(s) defined.

Secondly, define the chain, by adding one or several steps, using the *Add step* option available from the table popup menu. According to the chosen level, the second signer will have to sign his chromatogram with the reason associated to this level, etc.

At each sign-off level, one or many reasons (for example x, y, z) can be specified in the *End level* column.

A level can be defined a single time as initial step.

The same level can be defined several times as final step.

If initial level and final level are identical, all the signatories that will sign since this level is reached will sign with the same level options.

If a final level does not correspond to the initial level of another step, it is the end of the signature chain.

Example 1:

Label	Mandatory comment	Level
Authorship	☑	1
Approval	☐	2
Responsibility	☐	3
Review	☑	4
Reject	☐	5
R1	☐	1
R2	☐	2
R3	☐	3
R4	☐	4
	☐	1

Begin level	End Level(s) (format : x,y,z)
Init	1
1	2
2	3,4
3	4,5
4	5

In this example, 9 reasons are configured: two for level 1, 2, 3, and 4 and one for level 5. Comment is mandatory for "Authorship" and "Review" reasons.

The administrator has defined the following sign-off reason chain:

First signer (Init): Must sign with a reason of level 1 (Authorship or R1).

Second signer: Must sign with a reason of level 2 (Approval or R2).

Third signer: Can sign with a reason of level 3 or 4 (Responsibility, R3, Review or R4).

Case 1: The third signer chooses a reason of level 3.

Fourth signer: Can sign with a reason of level 4 or 5 (Review, R4, Reject).

Case 1-1: The fourth signer chooses a reason of level 4:

Fifth signer: The fifth signer must sign with a reason of level 5 (Reject).

At this point, the chromatogram cannot be signed again.

Case 1-2**:** The fourth signer chooses a reason of level 5:

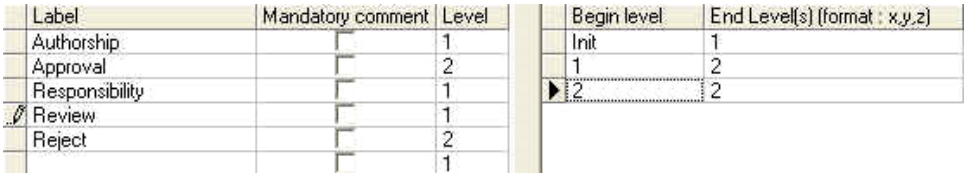
At this point, the chromatogram cannot be signed any more.

Case 2: The third signer chooses a reason of level 4.

Fourth signer: Must sign with a reason of level 5 (Reject).

The chromatogram cannot be signed again.

Example 2:



Label	Mandatory comment	Level
Authorship	☐	1
Approval	☐	2
Responsibility	☐	1
Review	☐	1
Reject	☐	2
	☐	1

Begin level	End Level(s) (format : x,y,z)
Init	1
1	2
2	2

In this example, five reasons are configured: three for level 1 and two for level 2. The administrator has defined the following sign-off reason chain:

First signer (Init): Must sign with a reason of level 1 (Authorship, Responsibility, Review).

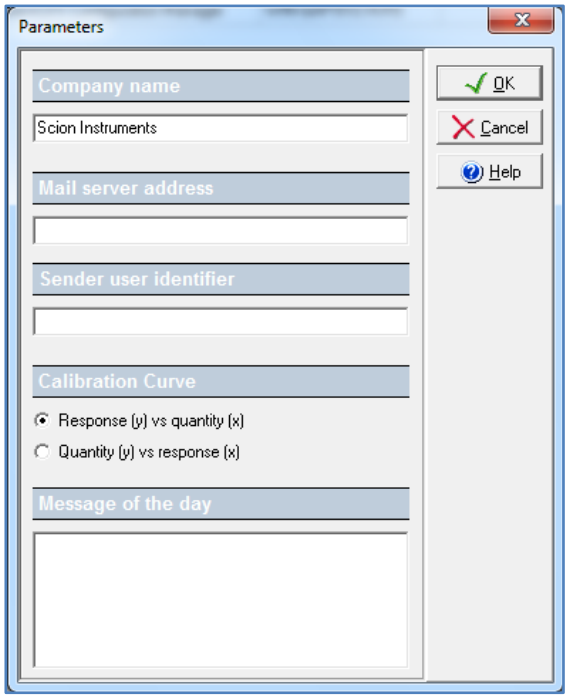
Second signer: Must sign with a reason of level 2 (Approval or Reject).

All the next signers must sign with a reason of level 2. The chromatogram can be signed an unlimited number of times

If no hierarchy is necessary, do not complete the table. Users can select any reason.

Parameters

Select the *CONFIGURATION / PARAMETERS* menu. The following screen is displayed:



The following options are proposed:

Company name: This field is informative; it allows naming of the company.

Mail server address: This field allows administrator to define the e-mail server address. This function is useful to notify administrator by e-mail in case of security event (lock of user or administrator account after the defined authorized number of consecutive unsuccessful attempts to log on). To realize this action, define the e-mail server address in the CONFIGURATION / PARAMETERS menu, then define the e-mail address of all administrators that must be advised of the security event, and possibly the '*Sender user identifier'* in the CONFIGURATION / PARAMETERS menu.

NOTE: All administrators that own an e-mail address are notified in case of security event. To not notify an administrator, do not define an e-mail address in its user properties.

Sender user identification: Enter in this field the text that will appear in origin from the e-mail sent if security event occurs.

Calibration curve: This function is very important; it allows definition of the calibration curve orientation used in CompassCDS, to quantify the sample.

Message of the day: The administrator defines in this field the text he wants to send to the users or administrators when they connect to a CompassCDS or a CompassCDS Configuration Manager session.

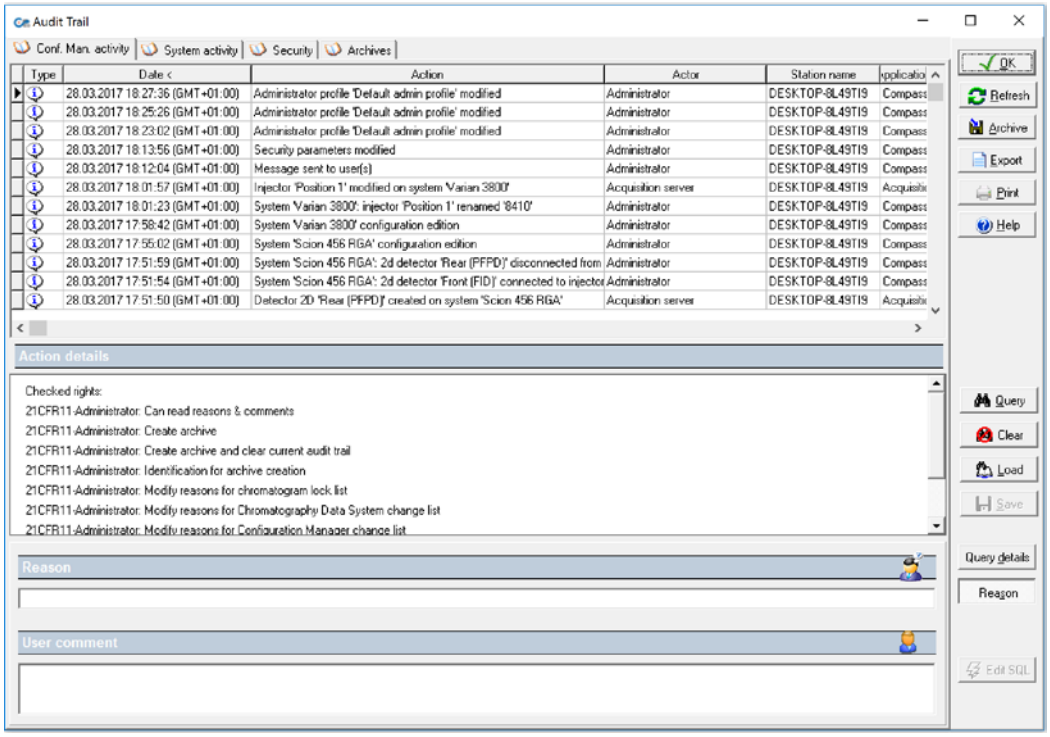
Audit Trail

This section of the software deals with all parameters relative to the Audit trail. It is based on the FDA 21-CFR11 rules, and provides a way to trace and view all the changes made in the CompassCDS Configuration Manager (create a project, delete a group, etc.), problems of security in CompassCDS Configuration Manager and in CompassCDS (failed connections, lock of stations or users, etc.), chromatographic system activity and provides a list of the audit trail archives.

To access the Audit Trail parameters, select the *AUDIT TRAIL* menu. The different options proposed are detailed bellow.

Current Audit Trail Viewing

To display the current Audit Trail, select the *AUDIT TRAIL / CURRENT AUDIT TRAIL* menu. The following screen is displayed:



The screen is divided into 4 tabs Conf*. Man. Activity, System activity, Security, Archives*. The content of each tab is detailed bellow. For each tab, the information displayed by action is: Type (information , warning or error), date, action, actor, station name, application.

Conf. man. Activity: This tab lists all the changes made in the CompassCDS Configuration Manager: Management of items (creation, deletion, modification, duplication, and associations), configuration parameters (password, security, electronic signature, licenses, content of audit trail etc.).

System activity: This tab lists all the starts and stops of chromatographic systems, made from CompassCDS Configuration Manager or CompassCDS.

Security: This tab lists all the parameters relative to connections (success and failure) to CompassCDS Configuration Manager or to CompassCDS, the lock of user account or stations due to error in connections, etc.

Archives: This tab lists the audit trail archive done from the software installation.

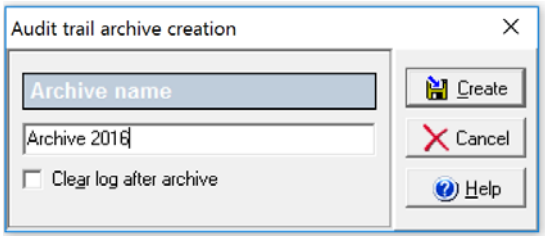
The Action details section gives the details of actions performed in case of *Conf. Man. Activity* tab selection.

A button list:

OK : To exit the screen.

Refresh : To display the changes made in the audit trail since the screen opening.

Archive : To archive the current audit trail. The administrator will have to identify itself before the archiving. Then the following screen is displayed:



Enter a name of the archived log in the *Archive name* field, define if you want or not to clear log after archiving.

If the option *Clear log after archive done* is selected, the *Current audit trail* screen will be cleared out in each tab except the *Archive* one that can never be empty.

If the option *Clear log after archive done* is not selected, the Archive action is specified in all the tabs of the *Current audit trail* screen.

NOTE: If the name given to the archive corresponds to an existing archive, a message is displayed enforcing administrator to change the name. It is indeed forbidden to overlay an existing archive log.

NOTE: It is strongly advised to archive and clear regularly the Audit trail, to avoid having a too large size audit trail file.

Export : To export the selected audit trail tab content in HTML format. If a query is performed the result of the query is exported.

Print : To print the selected audit trail tab content. If a query is performed the result of the query is printed.

Help : To access the on-line help.

NOTE: Only the administrators that are assigned the corresponding right (admin profile) can: archive the audit trail, clear the log after archive or print the audit trail.

Query: To realize a query on the selected Audit Trail tab.

Clear: To cancel the query and recover the complete Audit Trail.

Load: To load a saved query and apply it again.

Save: To save the defined query.

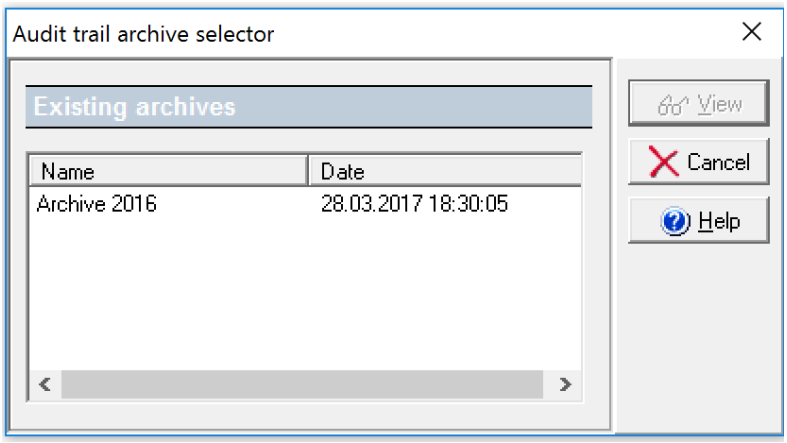
Query details: To display the query definition on the screen.

Reason: To display the reason and comment defined when the change was performed. The entry of mandatory reason and comment has to be defined in the admin profile.

Edit SQL: To define a query depending on a SQL script.

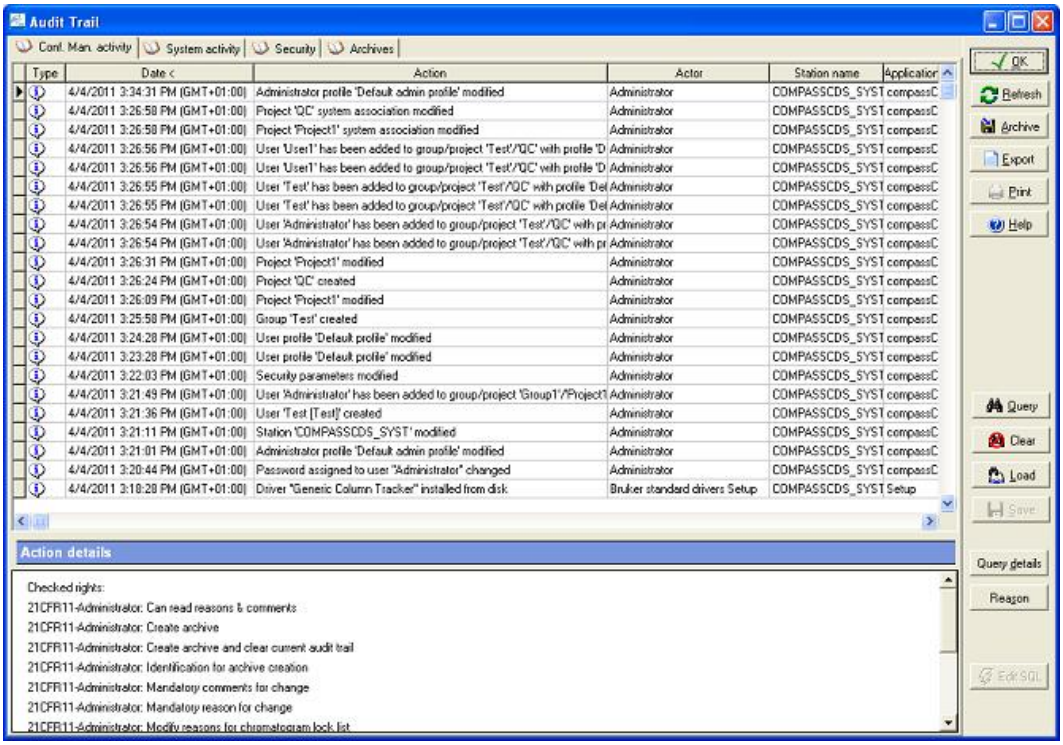
Archived Audit Trail Viewing

This option allows the administrator to view an archive of the audit trail. Select the *AUDIT TRAIL / AUDIT TRAIL ARCHIVE* menu. If archives exist, the following screen is displayed:



Select the line corresponding to the archive to display and click on the *View* button. The same screen as the one defined for the current audit trail is displayed, also displaying the name of the archive, and administrator who has created it, as well as the period covered. The administrator may print the archive.

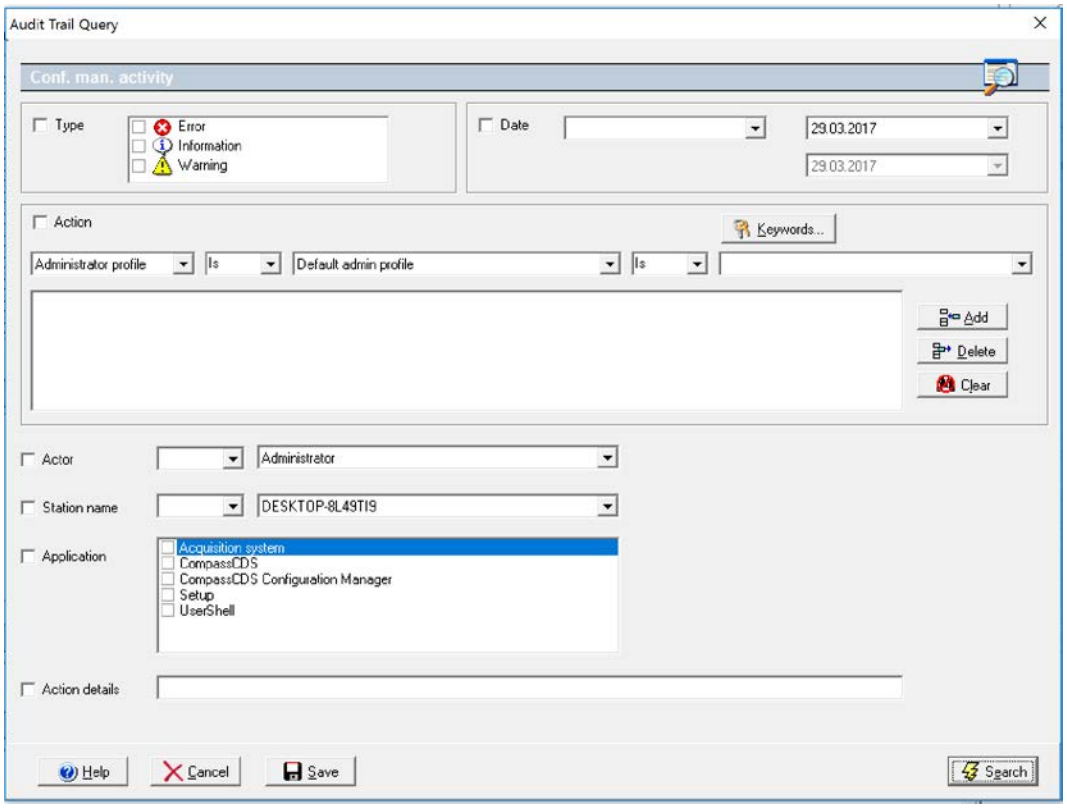
Audit Trail Query


Audit Trail
Conf. Man. activity
System activity
Security
Archives
Type
Date <
Action
Actor
Station name
Application
4/4/2011 3:34:31 PM (GMT+01:00) Administrator profile 'Default admin profile' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:58 PM (GMT+01:00) Project 'QC' system association modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:58 PM (GMT+01:00) Project 'Project1' system association modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:56 PM (GMT+01:00) User 'User1' has been added to group/project 'Test'/'QC' with profile 'D Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:56 PM (GMT+01:00) User 'User1' has been added to group/project 'Test'/'QC' with profile 'D Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:55 PM (GMT+01:00) User 'Test' has been added to group/project 'Test'/'QC' with profile 'Del Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:55 PM (GMT+01:00) User 'Test' has been added to group/project 'Test'/'QC' with profile 'Del Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:54 PM (GMT+01:00) User 'Administrator' has been added to group/project 'Test'/'QC' with pr Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:54 PM (GMT+01:00) User 'Administrator' has been added to group/project 'Test'/'QC' with pr Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:31 PM (GMT+01:00) Project 'Project1' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:24 PM (GMT+01:00) Project 'QC' created Administrator COMPASSCDS_SYST compassC
4/4/2011 3:26:09 PM (GMT+01:00) Project 'Project1' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:25:58 PM (GMT+01:00) Group 'Test' created Administrator COMPASSCDS_SYST compassC
4/4/2011 3:24:28 PM (GMT+01:00) User profile 'Default profile' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:23:28 PM (GMT+01:00) User profile 'Default profile' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:22:03 PM (GMT+01:00) Security parameters modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:21:49 PM (GMT+01:00) User 'Administrator' has been added to group/project 'Group1'/'Project1' Administrator COMPASSCDS_SYST compassC
4/4/2011 3:21:36 PM (GMT+01:00) User 'Test [Test]' created Administrator COMPASSCDS_SYST compassC
4/4/2011 3:21:11 PM (GMT+01:00) Station 'COMPASSCDS_SYST' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:21:01 PM (GMT+01:00) Administrator profile 'Default admin profile' modified Administrator COMPASSCDS_SYST compassC
4/4/2011 3:20:44 PM (GMT+01:00) Password assigned to user "Administrator" changed Administrator COMPASSCDS_SYST compassC
4/4/2011 3:18:28 PM (GMT+01:00) Driver "Generic Column Tracker" installed from disk Bruker standard drivers Setup COMPASSCDS_SYST Setup
OK
Refresh
Archive
Export
Print
Help
Query
Clear
Load
Save
Query details
Reason
Edit SQL
Action details
Checked rights:
21CFR11-Administrator: Can read reasons & comments
21CFR11-Administrator: Create archive
21CFR11-Administrator: Create archive and clear current audit trail
21CFR11-Administrator: Identification for archive creation
21CFR11-Administrator: Mandatory comments for change
21CFR11-Administrator: Mandatory reason for change
21CFR11-Administrator: Modify reasons for chromatogram lock list

Queries can be performed on the current Audit trail or on an archived Audit trail, to allow easy recovery of information.

The editing of query in the Audit Trail is guided, to make it easy to build. To define a query, open the current audit trail or an archive, select the tab on which query has to be build and press the

button. The following screen is displayed:



A query can be composed of different requests concerning the different columns of the Audit Trail (*Type, Action, Actor, Station name, Application* and *Action details* if the query is done on the Conf.Man.Activity tab). Requests are separated by a AND logical operand.

First select the parameter (column name) to add to the query by checking the associated check box, and then define the content of the request. For example check the *Date* check box, and then select the operator in the scrolling list and the date using the calendar. Operators proposed are: IS to select an item in a scrolling list, or CONTAINS to define manually the item in the field. The CONTAINS operator allows you, for example, to define a query on a deleted item, that will not be proposed in the scrolling list.

The *Action* section is a little more elaborated, and allows the administrator to define several requests on the *Action* column of the Audit Trail separated by an OR operand. For example the user wants to display all actions about modification of the group GROUP1 (request 1) OR all actions about the deletion of users (request 2). The way to process is to build the request 1, click on the Add button, then define the request 2 and click on the Add button. The final request is displayed in the dedicated field. To delete one of the requests, select it and click on the Delete button. To clear all the requests on the Action, click on the Clear button. An Action request can be more or less accurate and customizable, using the Keywords option that allows you to select predefine keywords or create new ones. You can indeed realize a query on Group only, by completing only the first scrolling list with Group; on a dedicated group, by defining the request as followed: ‘group’ is ‘GROUPNAME’; or on the creation of a dedicated group for example by defining the request as followed: ‘group’ is ‘GROUPNAME’ is ‘created’. If those criteria are not accurate enough, you can complete the *Action details* section. This section is not assisted; you have to enter manually the keyword(s) in the dedicated field. The SQL programming language can be used in this field.

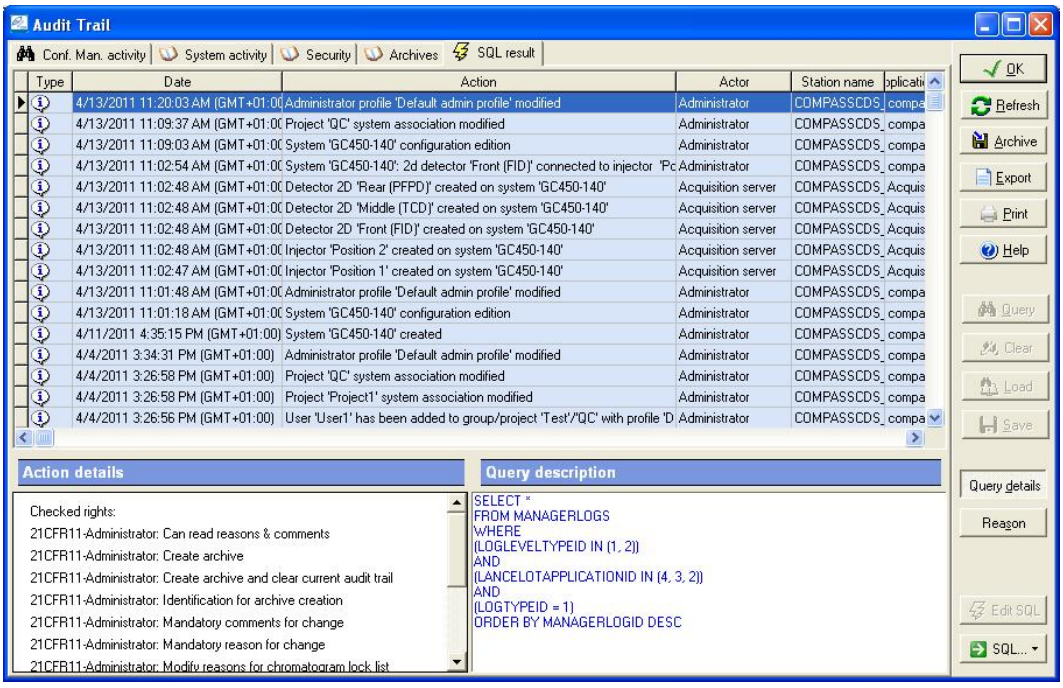
NOTE: The words used to define the query represent the words displayed in the Audit Trail, so the spelling and the order are important. So if you define Keywords (either in *Action* or *Action details*), be sure those words are used in the action column of the Audit trail.

Once the query is defined, press the Search button. The result of the query is displayed on the corresponding tab. Only lines satisfying the query are displayed.

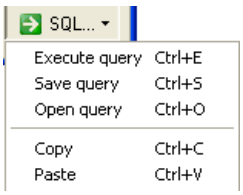
To save the query for a next research, press the Save button, and give a name to the query.

To cancel the query, press the Cancel button, to access the on-line help press the Help button.

For an advanced use of the query, it is possible to define a query by using a SQL script. Once a query is applied, the Edit SQL button is available. Clicking on it displays another tab named *SQL result* in the audit trail screen, converts the Query description in SQL language and adds the SQL... button:


Audit Trail
Conf. Man. activity
System activity
Security
Archives
SQL result
Type
Date
Action
Actor
Station name
4/13/2011 11:20:03 AM (GMT+01:00) Administrator profile 'Default admin profile' modified
4/13/2011 11:09:37 AM (GMT+01:00) Project 'QC' system association modified
4/13/2011 11:09:03 AM (GMT+01:00) System 'GC450-140' configuration edition
4/13/2011 11:02:54 AM (GMT+01:00) System 'GC450-140': 2d detector 'Front (FID)' connected to injector 'Pc
4/13/2011 11:02:48 AM (GMT+01:00) Detector 2D 'Rear (PFPD)' created on system 'GC450-140'
4/13/2011 11:02:48 AM (GMT+01:00) Detector 2D 'Middle (TCD)' created on system 'GC450-140'
4/13/2011 11:02:48 AM (GMT+01:00) Detector 2D 'Front (FID)' created on system 'GC450-140'
4/13/2011 11:02:48 AM (GMT+01:00) Injector 'Position 2' created on system 'GC450-140'
4/13/2011 11:02:47 AM (GMT+01:00) Injector 'Position 1' created on system 'GC450-140'
4/13/2011 11:01:48 AM (GMT+01:00) Administrator profile 'Default admin profile' modified
4/13/2011 11:01:18 AM (GMT+01:00) System 'GC450-140' configuration edition
4/11/2011 4:35:15 PM (GMT+01:00) System 'GC450-140' created
4/4/2011 3:34:31 PM (GMT+01:00) Administrator profile 'Default admin profile' modified
4/4/2011 3:26:58 PM (GMT+01:00) Project 'QC' system association modified
4/4/2011 3:26:58 PM (GMT+01:00) Project 'Project1' system association modified
4/4/2011 3:26:56 PM (GMT+01:00) User 'User1' has been added to group/project 'Test'/'QC' with profile 'D
Administrator
COMPASSCDS
OK
Refresh
Archive
Export
Print
Help
Query
Clear
Load
Save
Action details
Query description
Checked rights:
21CFR11-Administrator: Can read reasons & comments
21CFR11-Administrator: Create archive
21CFR11-Administrator: Create archive and clear current audit trail
21CFR11-Administrator: Identification for archive creation
21CFR11-Administrator: Mandatory comments for change
21CFR11-Administrator: Mandatory reason for change
21CFR11-Administrator: Modify reasons for chromatogram lock list
SELECT *
FROM MANAGERLOGS
WHERE
(LOGLEVELTYPEID IN (1, 2))
AND
(LANCELOTAPPLICATIONID IN (4, 3, 2))
AND
(LOGTYPEID = 1)
ORDER BY MANAGERLOGID DESC
Query details
Reason
Edit SQL
SQL...

The administrator can then write a query in SQL language in the Query description field, then by selecting the SQL... button, the query can be executed or saved. This button also allows opening and copying and pasting of an existing query.



The table name to use is MANAGERLOGS, the fields to use in the script are listed below:

ManagerLogId: Primary key (integer), automatically incremented at each new line: if you sort the records with this field, it corresponds to the chronologic order.

LogTypeId: (Integer) Page: (1= Conf. man. Activity, 2=System Activity, 3=Security)

LogLevelTypeId: (Integer) Type (1=Information, 2=Warning, 3=Error)

LogDate: Date

TimeZone: (Integer) Time zone (GMT) (in minutes). For example 60 minutes in France.

StationName: Station name

UserName: Actor

Action: Action

Reason: Reason

Description: Action details

UserComment: User comment

Following are some script examples:

Getting all new audit trail lines made today (chronologic order):

```
SELECT *
FROM MANAGERLOGS
WHERE
LOGDATE BETWEEN CURRENT_DATE AND CURRENT_TIMESTAMP
ORDER BY MANAGERLOGID DESC
```

Getting all new audit trail lines made today by user 'ADMINISTRATOR' in chronological order:

```
SELECT *
FROM MANAGERLOGS
WHERE
USERNAME = 'ADMINISTRATOR'
AND
LOGDATE BETWEEN CURRENT_DATE AND CURRENT_TIMESTAMP
ORDER BY MANAGERLOGID DESC
```

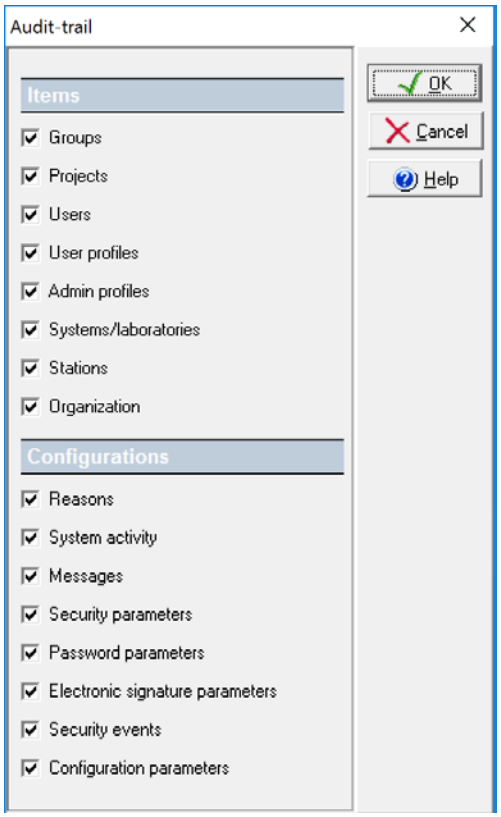
```
SELECT *
FROM MANAGERLOGS
WHERE
USERNAME = 'ADMINISTRATOR'
AND
LOGDATE BETWEEN CURRENT_DATE AND CURRENT_TIMESTAMP
```

Getting all new audit trail lines made by users 'ADMINISTRATOR' OR ‘JANE BURTON’ and concerning the Configuration Manager activity in chronological order:

```
SELECT *
FROM MANAGERLOGS
WHERE
USERNAME IN ('ADMINISTRATOR', 'JANE BURTON')
AND
(LOGTYPEID = 1)
ORDER BY MANAGERLOGID DESC
```

Configuration of Audit Trail content

This option allows the administrator configuring the actions to login the audit trail. Select the *AUDIT TRAIL / CONFIGURE AUDIT TRAIL* menu, the following screen is displayed:



The administrator must select the parameters to log in the audit trail. For example, to display all actions performed on user (creation, modification, deletion, association, duplication), the *Users* option must be selected.

NOTE: All changes made in this screen are compulsorily logged in the audit trail.

Reason configuration

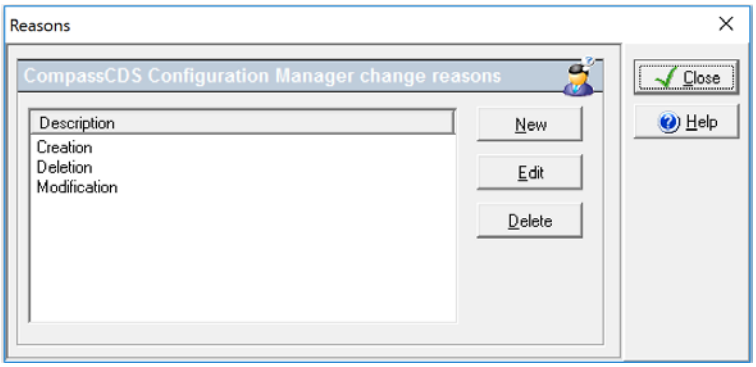
This option allows the administrator configuring the reasons to propose to user when realizing changes both in CompassCDS Configuration Manager and in CompassCDS. Select the *AUDIT TRAIL / CONFIGURE REASONS* menu, and then select the type of reason to configure:

CompassCDS Configuration Manager changes: Reasons proposed for changes realized in the CompassCDS Configuration Manager.

CompassCDS changes: Reasons proposed for changes realized in CompassCDS.

CompassCDS locks: Reasons proposed for chromatogram lock/unlock realized in CompassCDS.

For the three available types of reason, the same type of screen is displayed:



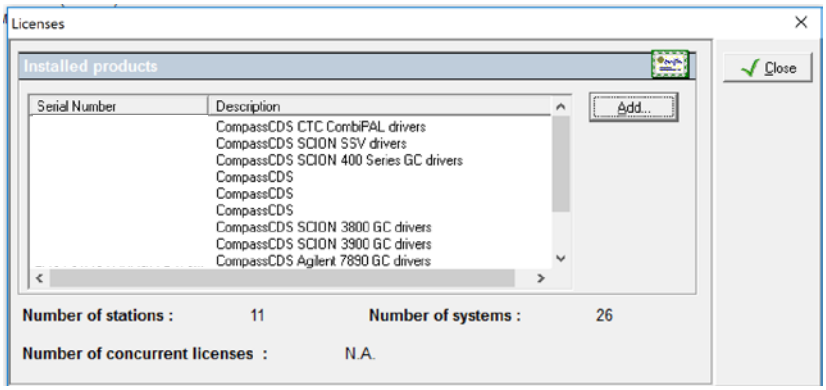
Administrator can add a new reason, remove or modify a selected reason.

Options

Licenses

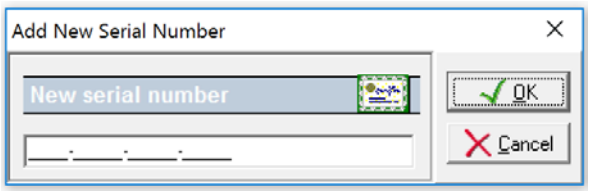
Licenses allow the administrator to manage the number of chromatographic systems and instrument drivers. According to the customer needs, several licenses may be installed.

Select the *OPTIONS/ LICENSES* menu, the following screen is displayed:



In the *Installed products* section, the administrator can consult the licenses serial number he has installed. He can also add new license(s) to modify the number of authorized systems or add new instrument drivers. The number of stations and systems authorized is updated and displayed at the bottom of the screen in real time.

To add a new license, click on the *Add* button, the following screen is displayed.



Enter the new serial number and validate by *OK*. The added serial number is listed in the main window.

Devices

The *OPTIONS / DEVICES* menu allows service people to install or update drivers with prerelease or beta drivers for testing. This functionality cannot be used by customer. This menu is displayed only if the corresponding right is selected in the Admin profile.

Lock Connection

This function can be used in a maintenance operation to forbid new connections.

To reactivate the connection, the administrator must select again the *OPTIONS / LOCK CONNECTION* option.

NOTE: Others fields like the BootP options are potentially displayed in the OPTIONS menu.

View

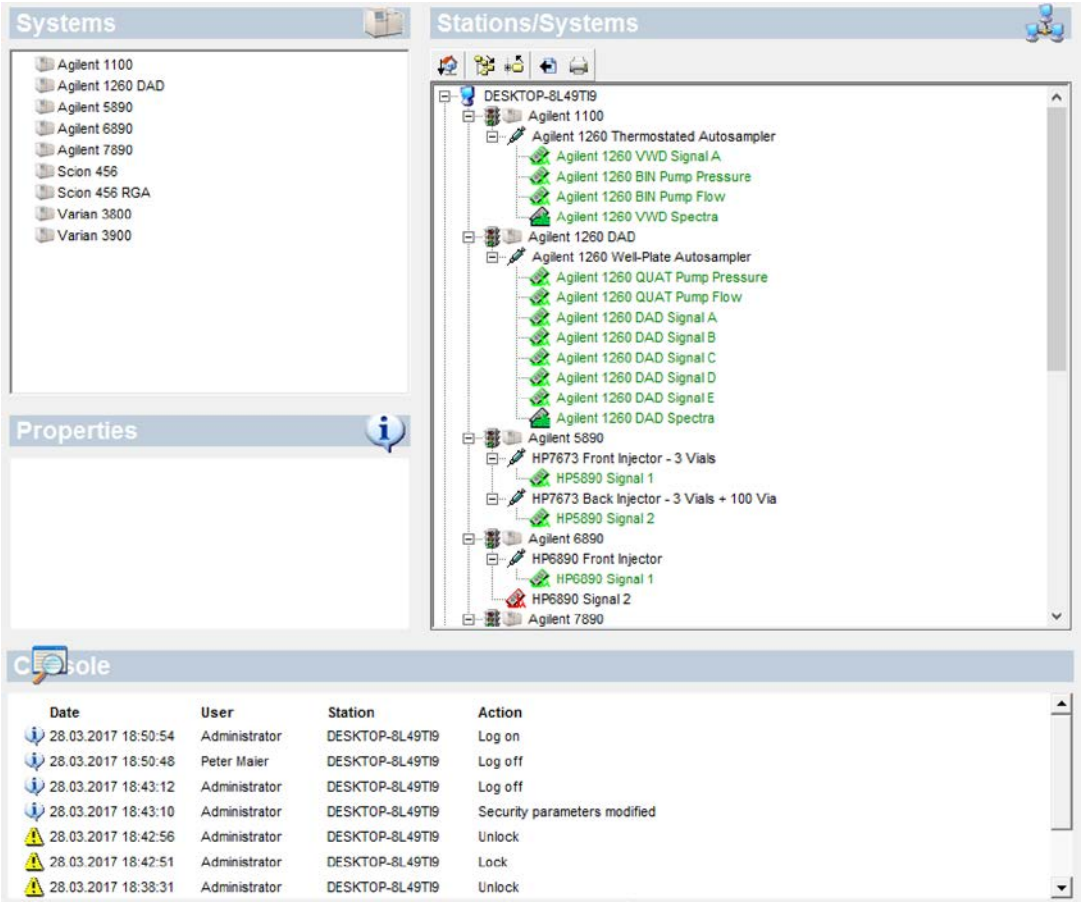
Refresh

This option allows the administrator refreshing the database. Note that just the system status, the console and the changes made by the connected administrator are refreshed in real time.

The user knows when a refresh of database is needed as the symbol of the Refresh icon becomes red ( ) and as a message “Please refresh the base (press F5)” is displayed at the bottom of the main screen.

Show Console

This option allows the administrator displaying the last actions logged in the audit trail in the main screen of the Configuration Manager, to be advised in real time of the actions performed by another administrator logged in the same time in another CompassCDS Configuration Manager session. Select the *VIEW / SHOW CONSOLE* menu, the following screen is displayed:



The number of actions to list in the console has to be set in the Preferences (*FILE / PREFERENCES*).

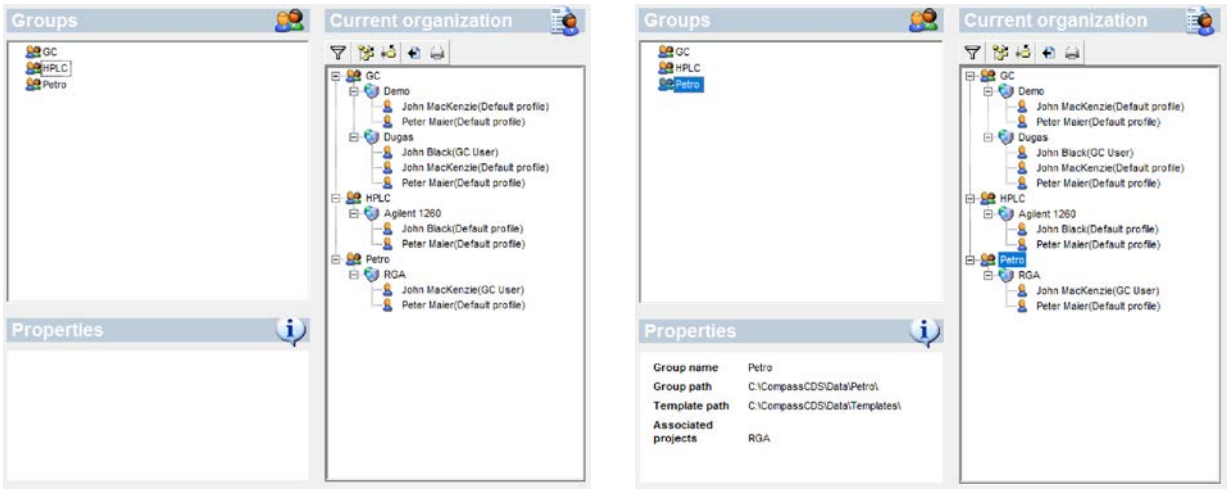
NOTE: To deactivate the console display, select again the *Show console* option in the *VIEW* menu.

Show Properties

This option allows the administrator displaying the properties panel when it is checked in the *VIEW / SHOW PROPERTIES* menu.

Groups

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Groups panel in the left top part of the main screen.



Projects

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Projects panel in the left top part of the main screen.

Users

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Users panel in the left top part of the main screen.

User profiles

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the User profiles panel in the left top part of the main screen.

Admin profiles

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Admin profiles panel in the left top part of the main screen.

Stations

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Stations panel in the left top part of the main screen.

Systems

This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Systems panel in the left top part of the main screen.

Connections

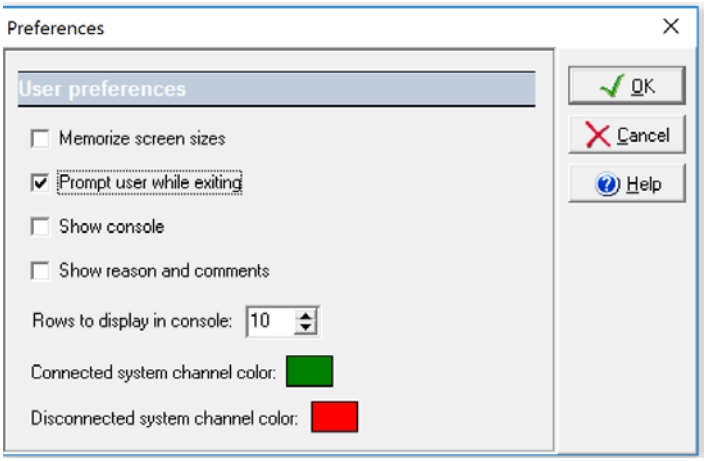
This option, when it is selected, modifies the main screen organization and leads to the immediate displaying of the Connections panel in the main screen.

File

Preferences

This option allows configuring some parameters that are administrator dependent and that will be taken into account only when the corresponding administrator is logged.

Select the *FILE/ PREFERENCES* menu, the following screen is displayed:



Memorize screen sizes: The sizes of the three main screens of the CompassCDS Configuration Manager are memorized if this option is checked and are applied at each new connection to the CompassCDS Configuration Manager.

Prompt user while exiting: A message is displayed when exiting the CompassCDS Configuration Manager if this box is ticked.

Show console: The console is automatically displayed at new connections to the CompassCDS Configuration Manager if this option is selected. The number of actions to list in the console is set in the *Rows to display in console* field (from 1 to 999). The default value is 10.

Show reason and comments: The reason and comments are automatically displayed when opening the audit trail.

Connected system channel color: Allows the administrator to change the color of the detector channels that are connected to injectors in the stations/systems view. The default color is green.

Disconnected system channel color: Allows the administrator to change the color of the detector channels that are disconnected from the injectors in the stations/systems view. The default color is red.

Quit

This option leads to the closing of the CompassCDS Configuration Manager session.

Help

Help

This option allows the administrator accessing the on-line help.

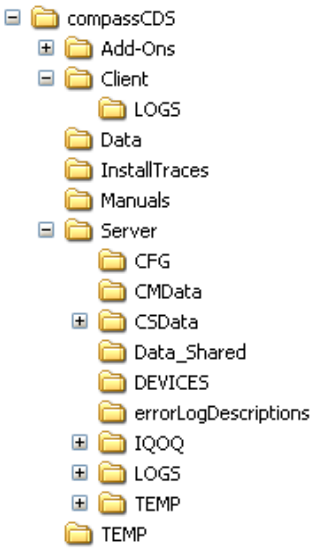
About

This option allows the administrator accessing the software information screen.

CompassCDS File Management under Windows

This part describes the content of the CompassCDS directory, created during the software installation, and gives some information about the main files.

The CompassCDS directory content is accessible from the Windows explorer:



The Add-Ons directory contains Plug-Ins and Tools.

- The Client directory contains:
  - CompassCDS.exe, the CompassCDS executive file
  - CompassCDS report Editor.exe, the CompassCDS report manager executive file
  - CompassCDS and CompassCDS Report Editor Help files.
  - Functional files.
- The Data directory contains chromatogram examples and report style templates.
- The Manuals directory contains the CompassCDS installation guide, user guides for CompassCDS, CompassCDS Configuration Manager, CompassCDS report Editor & CompassCDS print manager.
- The InstallTraces directory contains a report listing all the actions done during the installation of CompassCDS and the migration log file.
- The Server directory contains:
  - ConfigManager.exe: The CompassCDS configuration and maintenance manager executive file.
- CFG directory contains the configuration of all declared chromatographic systems.
- CMData directory contains database tables with all the CompassCDS configuration information (groups, projects, users, stations, systems etc.) as well as lists of the options present in the user and admin profiles and the audit trails.
- Data_shared directory: This file contains the peak, group and chromatogram formats defined in CompassCDS. Chromatogram annotation formats own CRF extension, peak tables PKF and group tables GRF one. The .REPO files represent the repositories created in CompassCDS Chromatography Data System (variables creation). The .REGC files, created by user, contain all screen size configuration parameters (ex: main screen size, open file screen, etc.).
- Devices directory contains the installed control driver .dll files for all the declared chromatographic systems.
- Logs directory contains logs concerning the CompassCDS process (errors that occurred, list of the injections realized, etc.), a LogArchives subdirectory containing all the archives of CompassCDS Configuration Manager's audit trail created.

Glossary

Audit Trail: This is a function listing the history of an object, by specifying what change was made by which user and when.

Group: A group is a logical entity, for example it is possible to have a QC group, a research group, etc. Depending upon the configuration, a group can also be a product name, or type of analysis such as LC or GC. Each group can have its own shared data such as method or report style. An unlimited number of groups can be created within CompassCDS

Project: A project is a logical entity within a group. For example, inside the QC group, different projects such as molecular analysis or techniques can exist. Each project can have its own shared data such as method or report style. An unlimited number of projects can be created for each group within CompassCDS.

User: A user is a physical entity, and must be associated to a project within a group. Users will have certain specific rights. The user who is a member of Project P1 inside Group G1 is not necessarily a member of project P1 inside Group G2.

Profile: A profile is the set of rights assigned to a user. User access to software features may be allowed or dis-allowed his/her profile. A profile is assigned to a user within a group and this means that if the user is associated with several projects in the same group, he/she will keep the same profile in each one of these projects. Nevertheless, a user can also have profile PR1 inside P1/G1, and another, different, profile PR2 inside P1/G2 if this is a requirement.

Station: A station is a physical computer connected to CompassCDS.

System: A system is a logical entity comprising at least one injector and one or more channel (detector) objects and which can include multiple physical devices.

CompassCDS
Column and Solvent Database Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501485
Revision D

Contents

Using the Column and Solvent Database Plug-in....3
Overview....3
Software functions....4
Chromatographic Column Management....4
Adding a New Column and Modifying Column Parameters....4
Managing the Columns List....6
Displaying Column Parameters....7
Displaying Column and Solvent Database Audit Trail....7
Chromatographic Solvent Management....9
Adding a New Solvent and Modifying Solvent Parameters....9
Managing the Solvents List....10
Displaying Solvents and Columns Database Audit Trail....10
Using the Generic Column Tracker Driver....11
Configuring the Generic Column Tracker....11
Building a Method....13
Control Method Section for the Generic Column Tracker....13
Starting and Viewing an Acquisition....14

Using the Column and Solvent Database Plug-in

This document describes the functions of the Column and Solvent Database Plug-in for CompassCDS.

Overview

The Column and Solvent Database Plug-in enables users to manage columns and solvents that are used in chromatographic systems. The columns and solvents and their properties are defined in a database that is available from CompassCDS. The Column and Solvent database is used for all chromatography types.

The Column and Solvent Database Plug-in permits users to automatically increment column parameters at each system injection. The Generic Column Tracker driver must be added as part of the configured system in CompassCDS and a column from the list must be selected in the method.

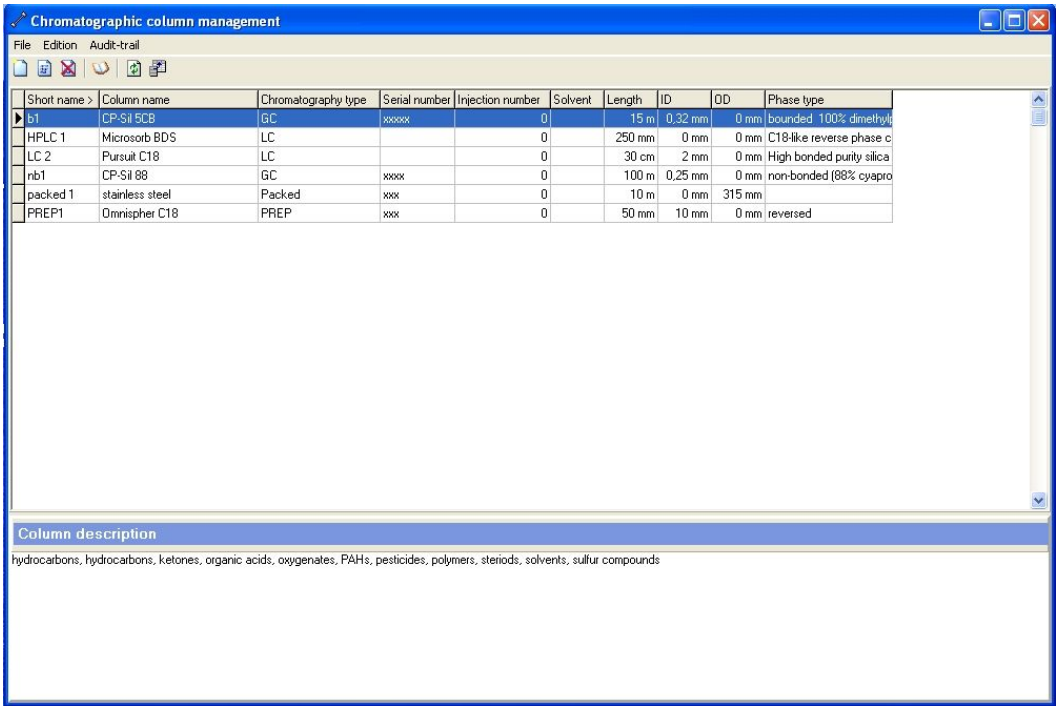
This plug-in can also manage solvent miscibility for Column Valve Modules.

A common audit trail lists all modifications in columns and solvents properties. The audit trail, the column and solvent properties and lists are exportable and printable.

Software functions

Chromatographic Column Management

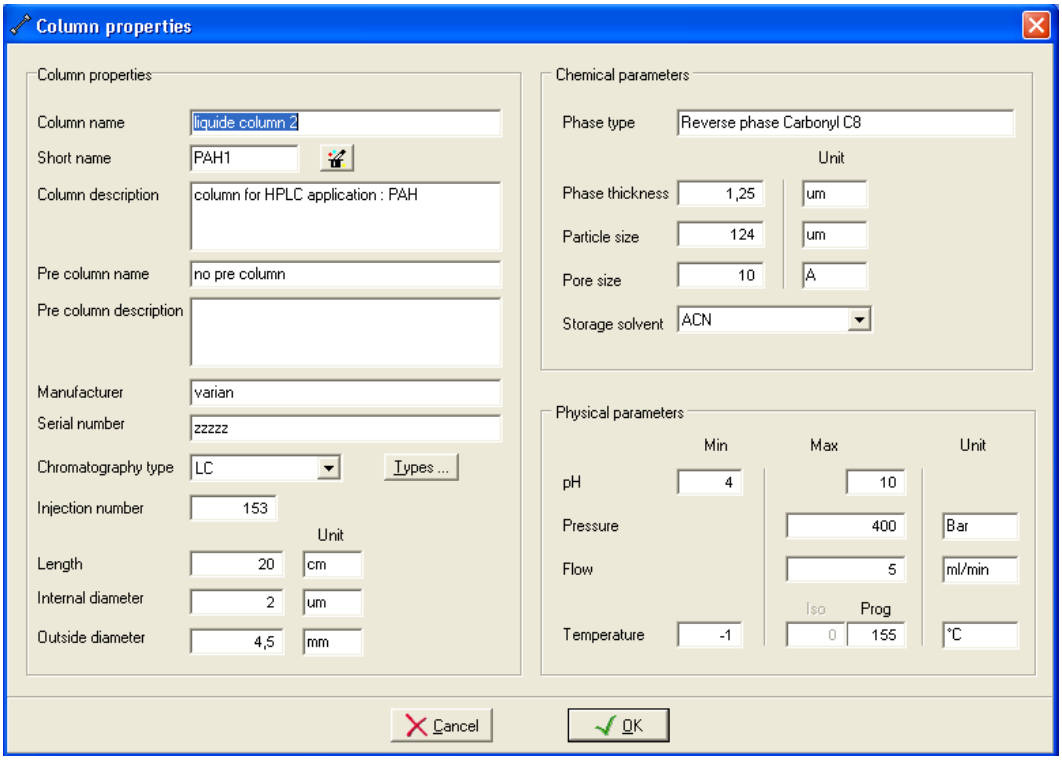
In CompassCDS, open the Chromatographic column management by selecting the icon or the corresponding option in the Plug-ins menu. The following screen is displayed:


Chromatographic column management
File Edition Audit-trail
Short name > Column name Chromatography type Serial number Injection number Solvent Length ID OD Phase type
b1 CP-Sil 5CB GC xxxxx 0 15 m 0,32 mm 0 mm bounded 100% dimethyl
HPLC 1 Microsorb BDS LC 0 250 mm 0 mm 0 mm C18-like reverse phase c
LC 2 Pursuit C18 LC 0 30 cm 2 mm 0 mm High bonded purity silica
nb1 CP-Sil 88 GC xxxx 0 100 m 0,25 mm 0 mm non-bonded (88% cyapro
packed 1 stainless steel Packed xxx 0 10 m 0 mm 315 mm
PREP1 Omnispher C18 PREP xxx 0 50 mm 10 mm 0 mm reversed
Column description
hydrocarbons, hydrocarbons, ketones, organic acids, oxygenates, PAHs, pesticides, polymers, steriods, solvents, sulfur compounds

It contains the list of all defined columns of the database. When selecting a column line, the Column description is displayed at the bottom of the screen.

Adding a New Column and Modifying Column Parameters

Define a new column in the column database by pressing the button, selecting ***EDITION / NEW*** menu or in the contextual menu. Modify the properties of a selected column by pressing, double-clicking, selecting EDITION / EDIT or in the contextual menu. Enter or modify the column parameters in the displayed column properties screen:



Only the column short name field need be completed, and all other fields are optional.

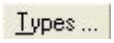
Validate the new settings by clicking on or cancel these.

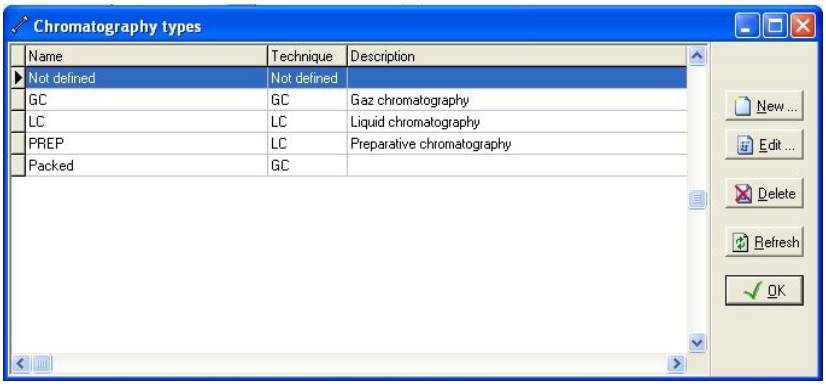
Column Properties Parameter Group

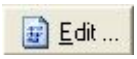
In the Column name field, enter the entire column name.

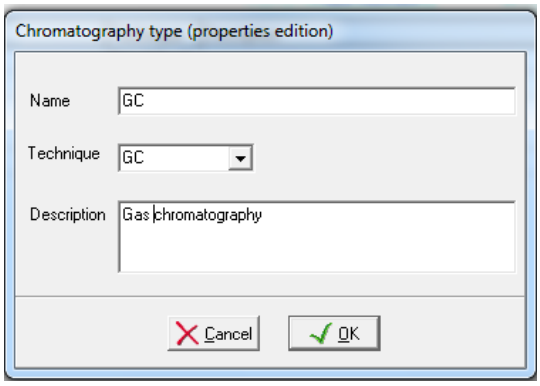
In the Short name field, enter a short name or click on the button to automatically define the 10 first characters of the Column name as Short name. The Short name is used for the CompassCDS column identification within a method and is mandatory.

Fill in the Column description, the Pre column name, the Pre column description, the Manufacturer name and the Serial number of the column.

Select the Chromatography type in the corresponding scrolling list. By default, GC, LC, PREP, Packed and Not defined are the available types. Press  to modify the chromatography types list. The following screen is displayed:



Press to add a new chromatography type and press  to modify the selected one. Choose the Technique and fill in the new Description and Name field in the displayed Chromatography type properties edition screen:



Validate the new settings by clicking on .

Press to delete the selected chromatography type and to refresh the list.

Fill in the column Length, Internal diameter, outside diameter and units in the corresponding fields.

Chemical Parameters Parameter Group

Enter the Phase type, Film thickness, Particle size, Pore size and units in the corresponding fields. Choose the Storage solvent among the whole Solvent database list.

Note that the Particle size, Pore size and Storage solvent fields are only available when the Chromatography technique is LC.

Physical Parameters Parameter Group

Enter the pH minimum and maximum values tolerated by the column in the Min and Max fields.

Enter the maximum Pressure and Flow with the units that the column can stand.

It is possible to fill in the pH and Flow fields only when the chromatography technique is LC.

Enter the column minimum and maximum temperatures when used in isothermal or programmed mode.

Managing the Columns List

Delete a selected column of the list by selecting the button, selecting EDITION / DELETE menu or from the contextual menu.

To duplicate a column entry in the list, select it and then the EDITION / DUPLICATE menu or from the contextual menu. A new column entry is created with exactly the same parameters except the Column name and the Short name. The column name of the created column entry begins with “copy of” and ends with the name of the duplicated column entry. The Short name of the created column entry corresponds to the first 9 characters of the duplicated Column name ended by a number suffix.

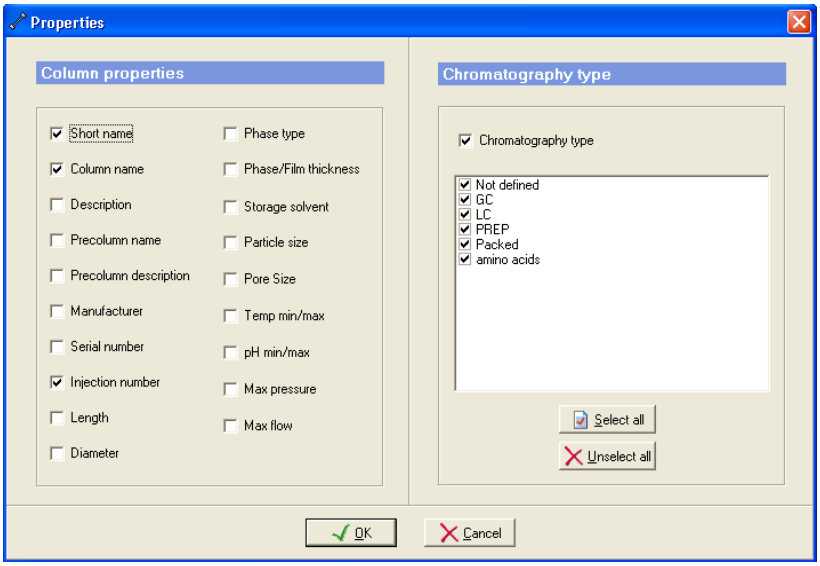
Print or Export in HTML the columns list by selecting EDITION / PRINT LIST or EDITION / EXPORT LIST. Choose the path to export and the file is automatically displayed at screen. The column parameters that are printed and exported are the currently displayed in the table and the Column description.

Print or Export in HTML each column parameters by selecting EDITION / PRINT PROPERTIES or EDITION / EXPORT PROPERTIES or from the contextual menu. Choose the path to export and the file is automatically displayed at screen.

Displaying Column Parameters

Click on the button to refresh the database as this can be modified from different stations at the same time, when in Client/Server configuration.

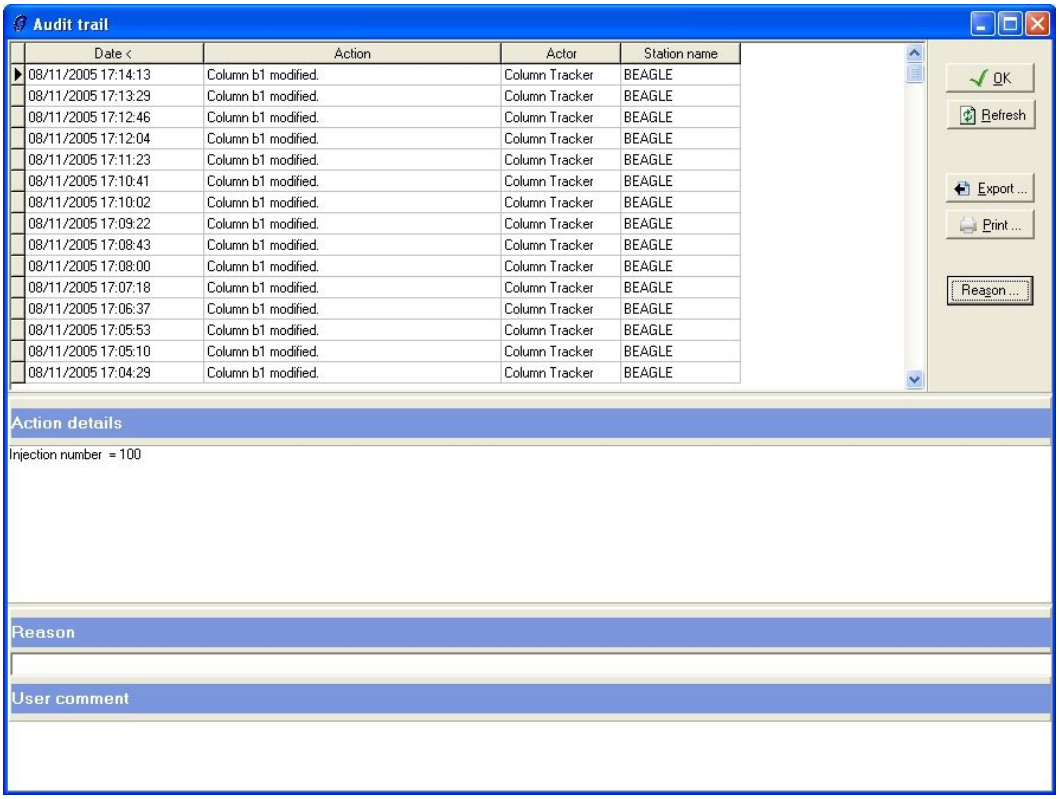
Click on the button or select Properties in the contextual menu to change the parameters to display in the column table. The following screen is then displayed:



To display a parameter in the column list table, check the corresponding box in the Column properties part. To display particular columns in the list depending on the type of chromatography, select that type in the Chromatography type section. Press Select all or Unselect all to select all available chromatography types or to unselect all checked types.

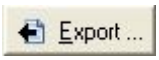
Displaying Column and Solvent Database Audit Trail

Press the button or select the AUDIT TRAIL / VIEW AUDIT TRAIL menu to display the column and solvent database audit trail.


Audit trail
Date <
Action
Actor
Station name
08/11/2005 17:14:13 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:13:29 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:46 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:04 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:11:23 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:41 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:02 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:09:22 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:43 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:00 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:07:18 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:06:37 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:53 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:10 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:04:29 Column b1 modified. Column Tracker BEAGLE
OK
Refresh
Export ...
Print ...
Reason ...
Action details
Injection number = 100
Reason
User comment

All modifications in the column parameters are listed in the audit trail with the corresponding date, actor and station. Each time an acquisition is done using a column that is defined in the Column and Solvent Database and in a system using the column tracker driver, the injection number of the column is automatically incremented in the column parameters. In that case, the actor listed in the audit trail is the name of the system and the system acquisition server is listed as station name.

Click on the button to refresh the audit trail.

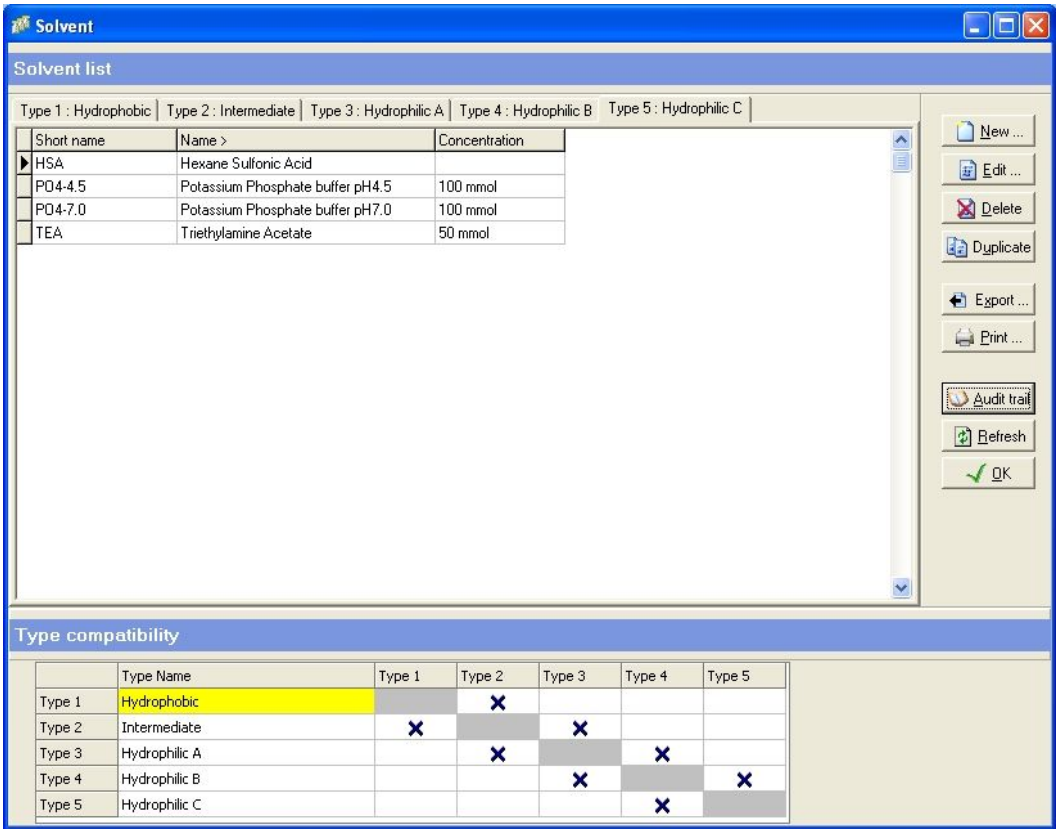
Click on the  button to export the current audit trail. Choose the export folder path and the file is automatically displayed at screen.

Click on the button to print the current audit trail.

Press the button to display user reasons and comments.

Chromatographic Solvent Management

In CompassCDS, open the Chromatographic Solvent Management by selecting the icon or the corresponding option in the Plug-ins menu. The following screen is displayed:

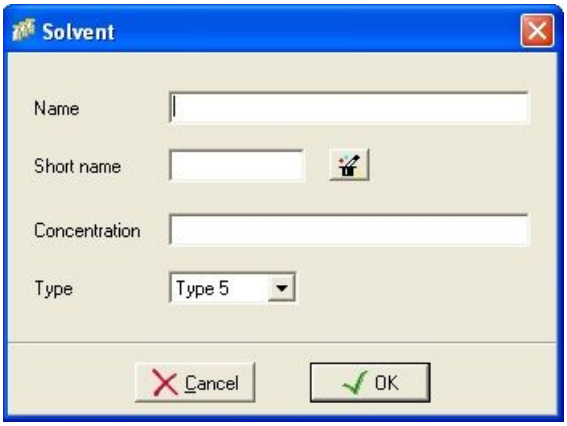


It contains the list of all defined solvents that are distributed into 5 different tabs depending on their hydrophobicity or hydrophilicity. Hydrophilic solvents are dispensed into three different types: the more hydrophilic corresponds to Type 5, the less hydrophilic to Type 3 and the moderately well hydrophilic to Type 4. The hydrophobic solvents are listed in the Type 1 tab and the solvents of intermediate hydrophobia in the Type 2 tab.

At the bottom of the screen, the Type compatibility table indicates the miscibility between solvents of different solvent types.

Adding a New Solvent and Modifying Solvent Parameters

Define a new solvent in the solvent type database by pressing the New ... button or from the contextual menu. Modify the properties of a selected solvent by pressing Edit ... or from the contextual menu. Enter or modify the solvent parameters in the displayed column properties screen:



Enter the solvent Name and Concentration.

In the Short name field, enter a short name or click on the button to automatically define the 10 first characters of the solvent name as Short name. The Short name is used for the CompassCDS solvent identification.

The solvent Name and Short name must be filled in.

Managing the Solvents List

Delete a selected solvent entry of the list by pressing the Delete button or from the contextual menu.

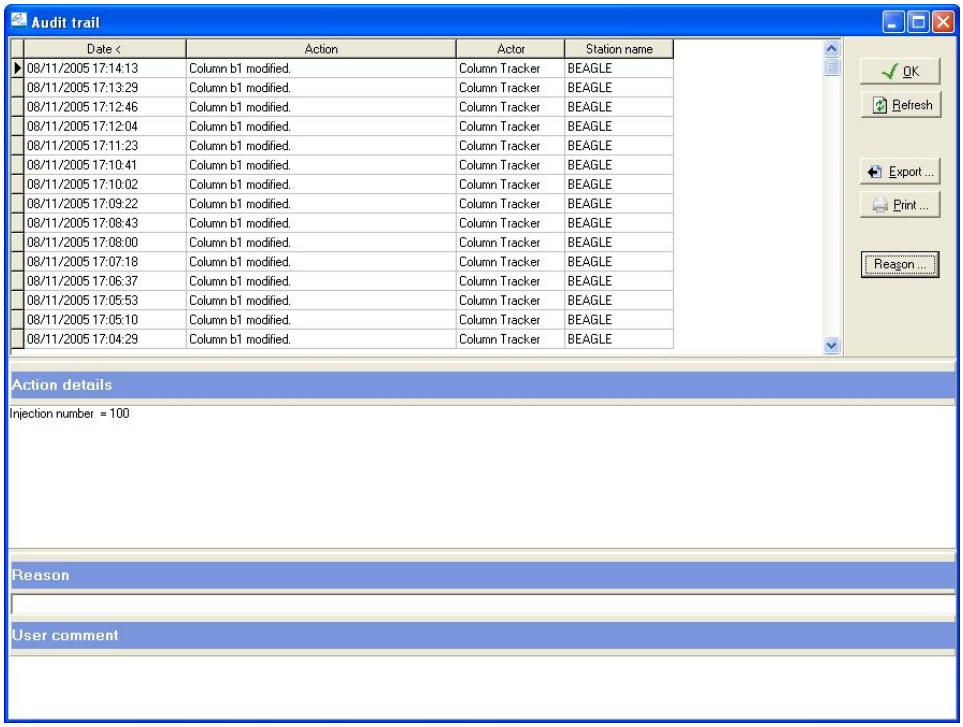
To duplicate a selected solvent entry in the list, press Duplicate or select it from the contextual menu. A new solvent entry is created with exactly the same parameters except the solvent *Name* and the *Short name*. The solvent *Name* of the created solvent entry begins with “copy of” and ends with the name of the duplicated solvent entry. The *Short name* of the created solvent entry corresponds to the first 9 characters of the duplicated solvent name ended by a number suffix.

Print or Export the solvent list and parameters by pressing the Print ... or Export ... button. Choose the path to export and the file is automatically displayed at screen.

Click on the Refresh button to refresh the database that can be modified from different stations at the same time, when in Client/Server configuration.

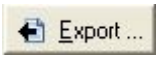
Displaying Solvents and Columns Database Audit Trail

Press the Audit trail button to display the column and solvent database audit trail.


Audit trail
Date <
Action
Actor
Station name
08/11/2005 17:14:13 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:13:29 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:46 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:04 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:11:23 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:41 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:02 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:09:22 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:43 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:00 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:07:18 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:06:37 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:53 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:10 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:04:29 Column b1 modified. Column Tracker BEAGLE
OK
Refresh
Export ...
Print ...
Reason ...
Action details
Injection number = 100
Reason
User comment

All modifications in the solvent parameters are listed in the audit trail with the corresponding date, actor and station.

Click on the button to refresh the audit trail.

Click on the  button to export the current audit trail. Choose the path to export and the file is automatically displayed at screen.

Click on the button to print the current audit trail.

Press the button to display user reasons and comments.

Using the Generic Column Tracker Driver

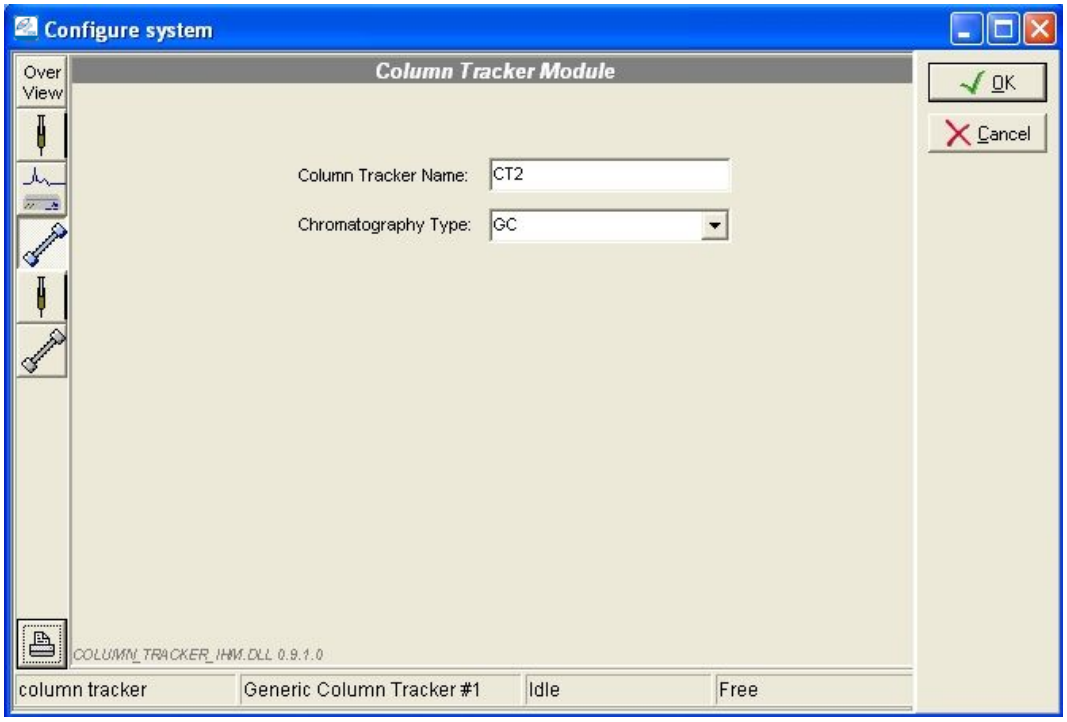
Use the Generic Column Tracker Driver in order to use the Column and Solvent Management Plug-in to automatically increment column parameters.

Configuring the Generic Column Tracker

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

NOTE: If the system is equipped with several columns, it is necessary that system driver list contains an equivalent number of instances of the column tracker driver as there are columns in the system.

Click on the button corresponding to the Generic Column Tracker driver and the configuration screen appears.



In cases where the system contains several columns, enter a Column Tracker Name to differentiate each column. This Column Tracker Name should be different for each Column tracker module of the system.

Choose the Chromatography Type of each column of the system in the corresponding scrolling list. All the defined chromatography types of the column database are available.

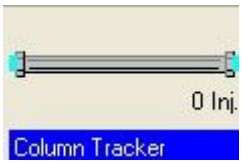
Configuring the Synopsis

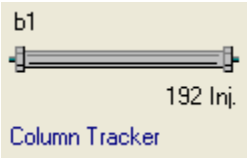
In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

The synopsis will be displayed in CompassCDS in the Systems tab. In this tab, the Overview will show the synopsis of the system.

For example, the following pictures represent the synopsis of the Generic Column Tracker:





NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration.

Building a Method

Create a new method for the system using the Generic Column Tracker driver.

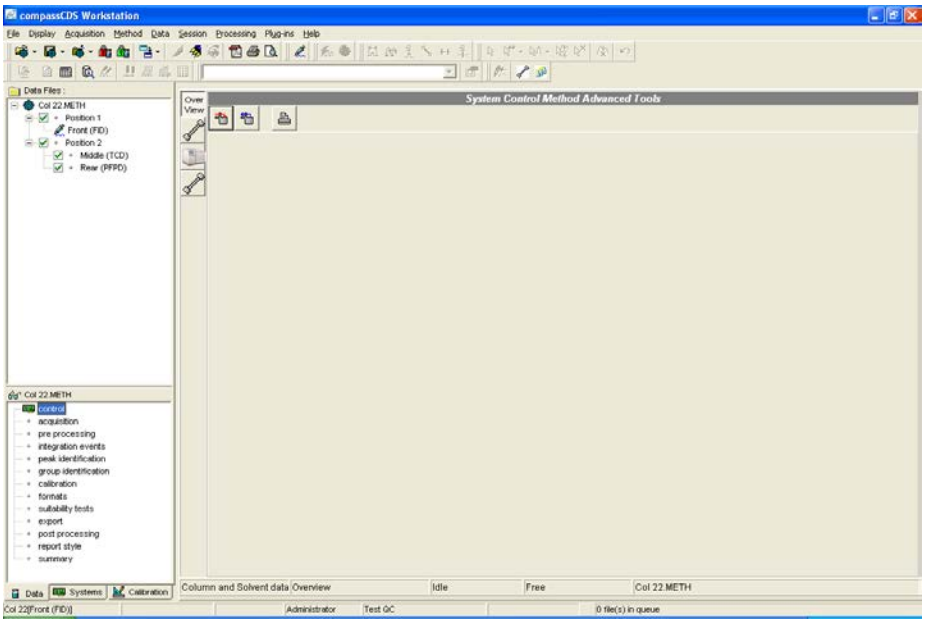
The control section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the Generic Column Tracker is described.

NOTE: For more details about the programming of each method section, consult the CompassCDS User Guide.

Control Method Section for the Generic Column Tracker

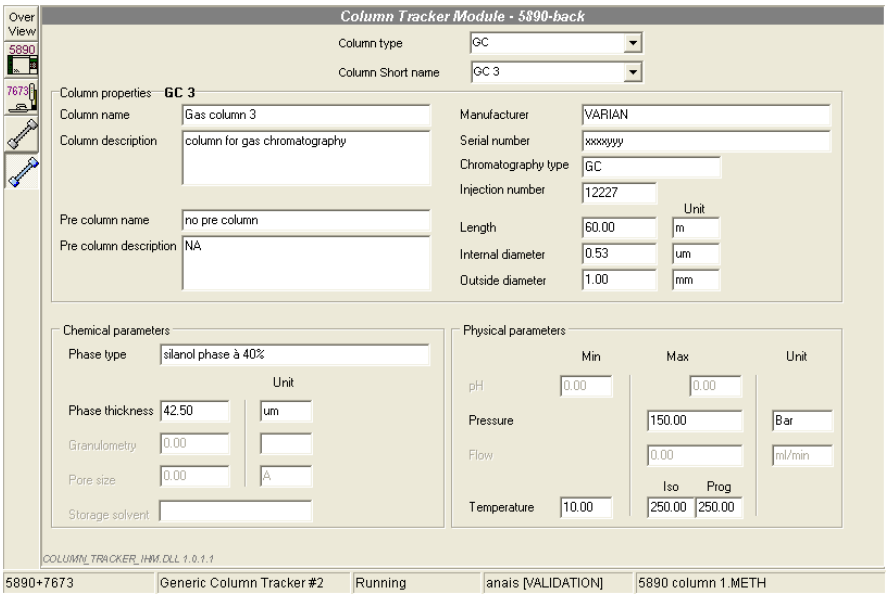
In the method, select the control section in the lower part of the browser.

The following screen appears:



Click on the button to display the Generic Column Tracker control method section.

Column Tracker Module Control



The Chromatography type chosen while configuring the system is displayed at the top of the control screen.

Select the Column Short name to be used in the system in the corresponding scrolling list just above. Only the columns defined for this Chromatography type are available in the scrolling list.

Once a column is selected, its Column properties, Chemical parameters and Physical parameters are automatically displayed on screen.

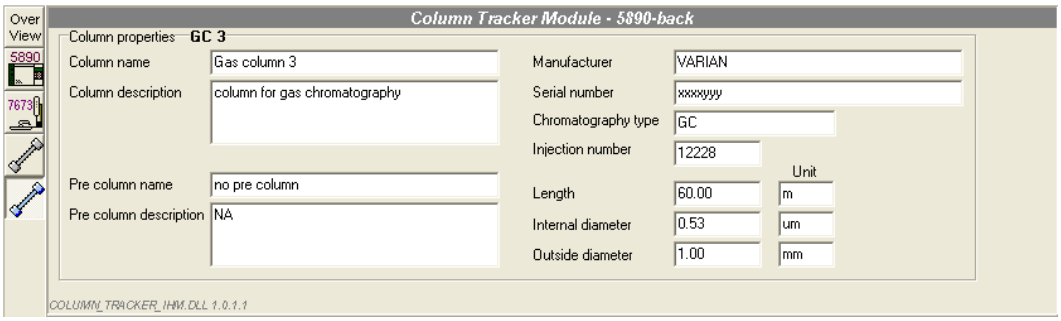
Starting and Viewing an Acquisition

To view a running acquisition, click on the Systems tab then select the running system.

Status of the Generic Column Tracker

Click on the button corresponding to the Generic Column Tracker driver and the Generic Column Tracker status screen will appear.

Status Window



The Status window displays the column properties as defined in the column database. All fields are in read-only mode. The Injection number is incremented at each injection.

CompassCDS
Print Manager Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501488
Revision D

Contents

Using Print Manager Plug-in 3
Overview 3
Software Functions 3
Direct PDF Export Tool 3
Print Manager Post-processing Tool 4

Using Print Manager Plug-in

This document describes the functions of the Print Manager Plug-in for CompassCDS.

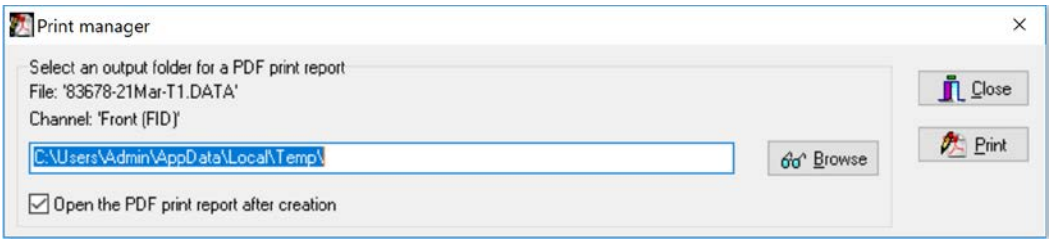
Overview

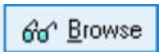
Print Manager Plug-in enables the user, when it is used as a post-processing application, to combine printing and export of the same chromatogram as a .PDF. Different printers, report styles and output paths can be selected in the same configuration table.

Software Functions

Direct PDF Export Tool

In CompassCDS, open the Direct PDF Export tool by selecting the icon or the corresponding option in the plug-ins menu. The following screen is displayed:



The user can select the path where the PDF export is going to be stored, via the 

button or just manually enter a path. The path can be a local path or one defined on a network disk. If this path is valid, it is saved and automatically displayed the next time this screen is accessed.

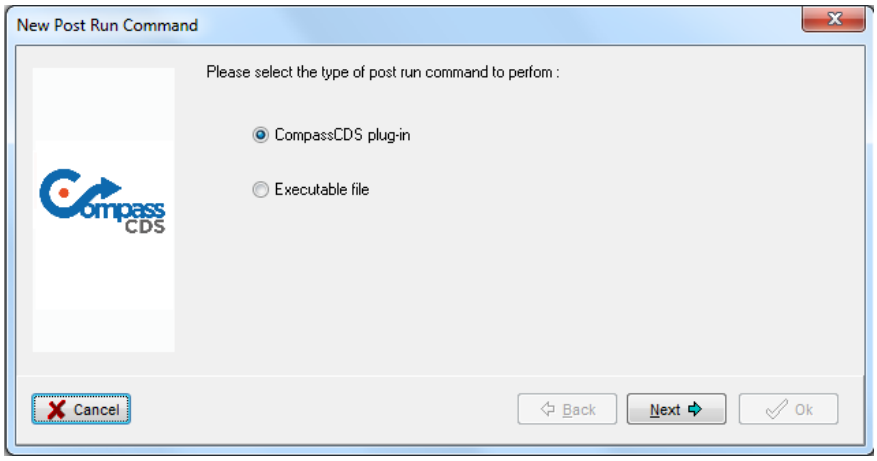
Once the export path is configured, it is possible to select the

button. The report style used for the creation of this PDF export is the report style defined in the report style section of the chromatogram's method. If no valid report style is defined, a warning message is displayed.

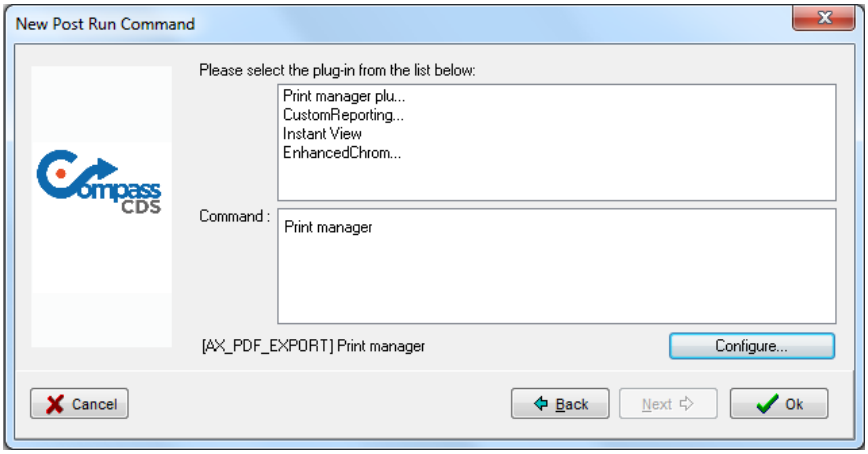
If the "Open the PDF print report after creation" box is checked, the PDF export is automatically displayed on the screen.

Print Manager Post-processing Tool

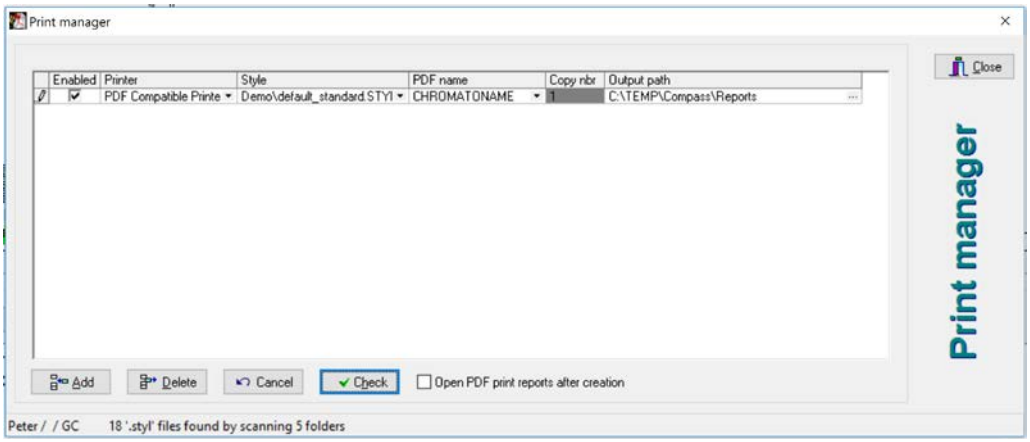
To configure the Print Manager tool in the post-processing part of the method, a user selects the Add... button and the selects the CompassCDS plug-in option in the following screen:



The Next button is selected followed by the Print Manager plug-in option shown in the following screen:



Select the Configure... button to access the configuration of the plug-in parameters.



A combination of printing and PDF export of the same chromatogram can be defined in this table. Different printers, report styles and output paths can be selected and added as additional lines

Normal printing

To configure normal printings, a pre-defined printer is selected in the Printer column. All the printers installed and configured on the computer are accessible.

One report style is selected from the list in the Style column. All the report styles that are stored in the connected group directory or in some group subdirectories are available. The total number of report styles found in the connected group directory is displayed at the bottom of the screen.

The number of print copies can be selected in the Copy number column

The output path is grayed in the case of normal printings.

PDF exports

To configure PDF exports, select the PDF Compatible printer driver in the Printer column.

Select one report style from the list in the Style column. All the report styles that are stored in the connected group directory or in some group subdirectories are available. The total number of report styles found in the connected group directory is displayed at the bottom of the screen.

Select one Global Variable from the list in the File Name column. This can be a System variable, a User Input or a User Formula. The DEFAULT value is: ‘CHROMATONAME’.DATA-‘CHANNELNUMBER’ ‘timestamp’

The corresponding Copy number cell is grayed as only a single PDF export can be done.

Select the path where the .PDF export is to be stored from the Output path column or simply enter it manually.

Additional lines can be added to this configuration table using the

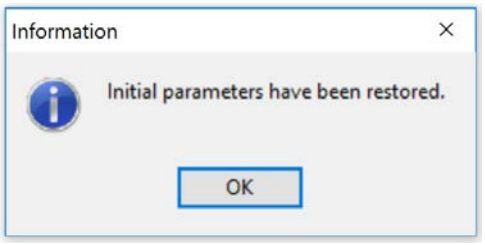
button.

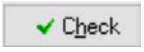
Lines can be removed from the configuration table using the

button.

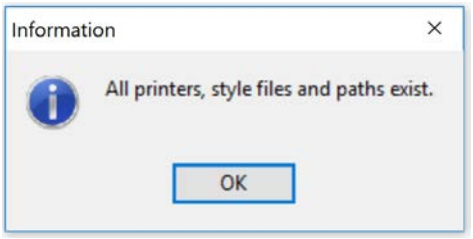
The last action can be cancelled via the

button and the previous parameters are restored. The following message is displayed at this time:

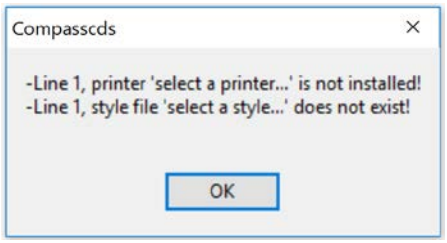


It is possible to verify that the defined report styles, printers and output paths really exist by selecting the 

button. If it is the case, the following message is displayed:



If one or more parameters are not valid, a message, similar to that shown below, is displayed



and the corresponding box in the Enabled column is automatically unchecked.

If the Open PDF print reports after creation box is checked, the created PDF exports are automatically displayed on the screen once created.

CompassCDS Report Editor User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501484
Revision D

Contents

Introduction 3
Application Details 4
- Working Environment 4
  - Toolbars 5
  - Browser 7
- Building the Report Style 7
- Object Properties 7
  - Graphic Object 7
  - Text Object 8
  - Label Object 9
  - Table Object 10
  - Chromatogram Object 11
  - Peak Results Object 13
  - Group Results Object 13
  - Method Object 14
  - Calibration Report Object 14
  - Suitability Tests Object 15
  - Electronic Signature Object 16
- Default Reports 16

Introduction

CompassCDS Report Editor enables you to create, customize, and print reports from the CompassCDS Chromatography Data System.

CompassCDS Reports may contain CompassCDS objects, such as Chromatograms, the Peak Report tables, any of the standard or custom variables, etc. A CompassCDS Report may also include Microsoft™ documents and other file types that include images and labels.

All of the objects can be places and sized within pages just as these are intended to be printed.

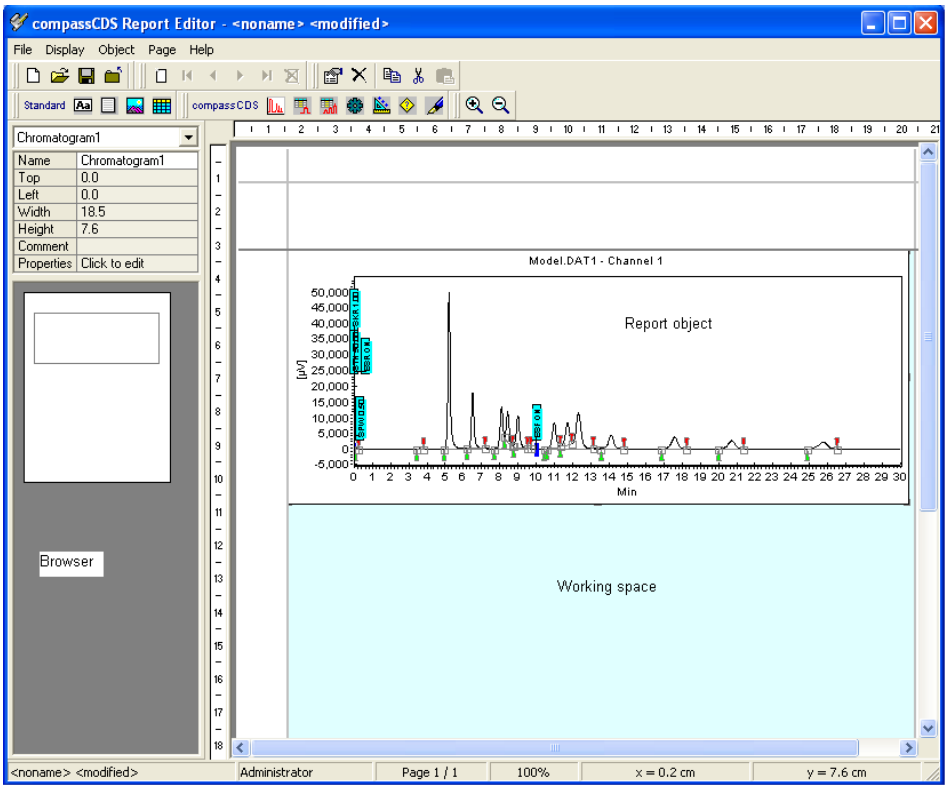
Application Details

The CompassCDS Report Editor enables a user to build customized reports.

For regulatory compliance, a report corresponding to an unsaved data file is printed with a ‘DATA NOT SAVED’ watermark in the background.

Working Environment

The CompassCDS Report Editor graphical environment is composed of a main menu, toolbars, a browser, a working space, and a status bar.



Main Menu

File	Used to manage the report style files (open, close, save, print).
Display	Allows a user to configure the zoom level, particularly the browser display.
Object	Allows a user to insert an object and edit its properties.
Page	This menu enables a user to define the page parameters.
Help	Enables access to the Help file and information about the CompassCDS Report Editor version.

File Menu

New style	Creates a new report style in CompassCDS Report Editor.
Open	Opens an existing report style.
Save	Saves the current report style.
Save as	Saves the current report style under a different name. (Note that ‘Save as’ will not allow a user to overwrite an existing file.)
Close	Closes the current report style.
Quit	Exits CompassCDS Report Editor.

Display Menu

Zoom in	Zooms in on the report.
Zoom out	Zooms out on the report.
Browser	Used to show or hide the browser enabling a user to see the contents of each page.

Object Menu

Insert	Inserts a CompassCDS object or a standard object. The available CompassCDS objects are a chromatogram, a peak or group result table, a method, a calibration report, a suitability tests, an electronic signature. The standard objects are a label, a graphic, a text (including CompassCDS variables), or a table. The corresponding object is always added in the left top corner of the page. Refer to “Building the Report Style” to learn how to resize or modify the position of a selected object.
Select	Selects an object.
Delete	Deletes the selected object.
Copy	Copies the selected object.
Cut	Cuts the selected object.
Paste	Inserts the contents of the clipboard.
Properties	Used to display and edit the properties of the selected object.

Page Menu

New Page	Creates a new page in the same report style. The new page is inserted before the active page.
New page at the end	Creates a new page at the end of the report.
Delete Page	Deletes the current page.
Page Break	Inserts a break between pages.
Next Page	Displays the next page.
Previous Page	Displays the previous page.
First Page	Displays the first page of the report.
Last Page	Displays the last page of the report.
Help Menu	
Help content	Displays the on-line Help.
About	Provides information about the CompassCDS Report Editor.

Toolbars

Several toolbars can be accessed from the Display menu

Pages Toolbar

This toolbar is useful if several pages have been defined:

Displays the first page of the report.

Displays previous page of the report.

Displays next page of the report.

Displays the last page of the report.

Adds a new page at the end of the report.

Deletes the current page.

Standard Toolbar

Creates a new report style.

Opens an existing report style.

Saves the current report style.

Closes the current report style.

Saves the current report style under a different name. (Note that 'Save as' will not allow a user to overwrite an existing file)

Used to cut the selected objects

Copies the selected object.

Inserts the contents of the clipboard.

Object Toolbar

This toolbar allows a user to add objects to the report style.

The corresponding object is always added in the left top corner of the page. Refer to "Building the Report Style" to learn how to resize or modify the position of a selected object.

Adds a label, for example the title of the report style, with a special display (colors, shadows, etc.).

Inserts a text object.

Inserts a graphic. Right-click on the graphic and select the image to be added in the report style.

Adds a table which is created and completed by the user.

Adds a chromatogram.

Adds a Peak Report, i.e., a table of the peaks in the chromatogram.

Adds a Group Report, i.e., a table of the groups in the chromatogram.

Adds the Method to the report. Press the right mouse button to choose which properties a user wants to print.

Prints the Calibration Curve.

Prints the Suitability Tests results.

Prints the Electronic Signature.

Displays the object properties.

Deletes the selected object

Display Toolbar

Zooms in on the report.

Zooms out on the report.

Browser

The browser is displayed on the left side of the screen and is divided into two sections.

The first section, (a table) shows properties of the selected objects (i.e., the object name, the location of this object in the page, a comment). Click on the Properties field to open the selected object properties.

The second section gives a preview of all pages of the report style. Clicking on any page displays it in the CompassCDS Report Editor.

Building the Report Style

To create a new report style from CompassCDS, a user selects the FILE / NEW / NEW REPORT STYLE menu: CompassCDS Report Editor is opened, and a blank report is displayed.

A report style is composed of several pages onto which objects (see below) are added. Each page is divided into a header area, a main area, and a footer area. The header and the footer are common and will be printed at the top and the bottom of all the pages.

The header and the footer areas are delimited with a line. The size of the header and footer can be modified. Clicking on the line modifies the cursor appearance and the line can be dragged to the desired location.

To place objects in the header, the main area, or the footer, the area is selected with the mouse, then the object is selected from the toolbar or from the insert menu.

The object is always added in the top left corner of the area. To move and resize the object a user can:

- click on the object and drag it to the desired location
- click on the grey squares and drag the borders of the object
- modify its coordinates in the browser

For each object, pop-up menus are made available by clicking the right mouse button. These pop-up menus enable access to functions such as delete, copy, cut, paste, and properties.

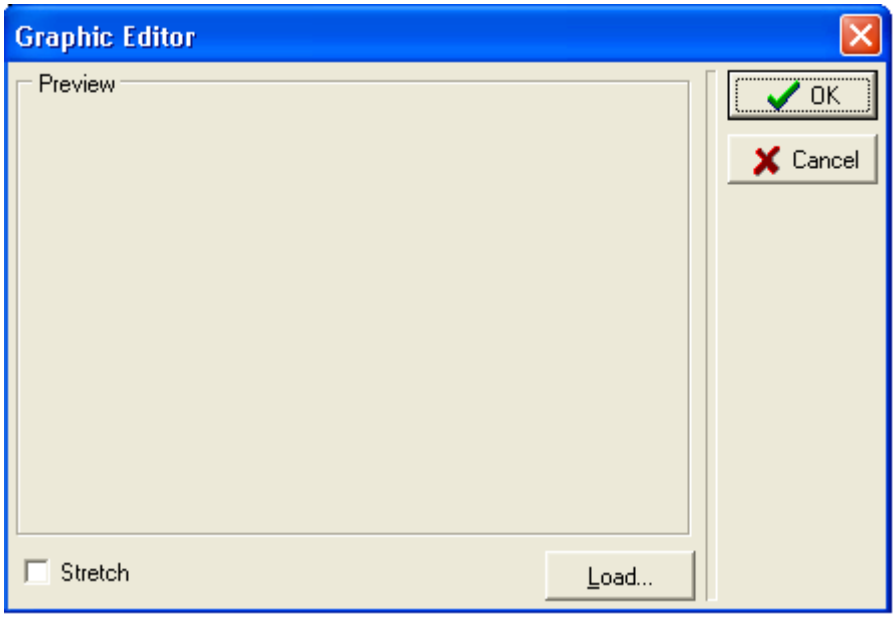
Object Properties

Once the object is added to the report, right-clicking on the object generates a pop-up menu a. Selecting the PROPERTIES menu option enables a user to configure the object.

Graphic Object

This object enables a user to display a graphic in bitmap format. It can be used to insert the company logo, for example.

In the pop-up menu selecting the PROPERTIES menu option enables a user to configure the object. The following window appears:

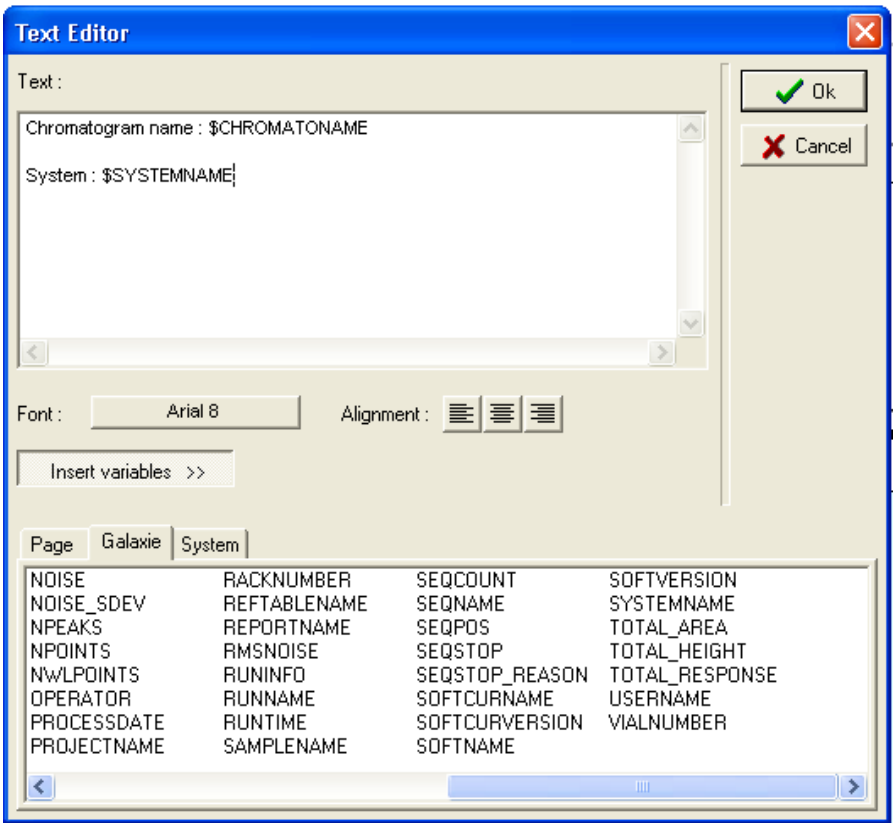


Pressing the Load button selects the image to display. A preview of the selected image is displayed.

Check Stretch to adjust the image to the object size.

Text Object

This object enables a user to enter text and variables in the report.



A variable name is always preceded by the symbol $.

A user may configure the font style, size, and color. The buttons modify text alignment.

Clicking on the Insert variables>> button enables a user to select one or more variables to display on a report. Three tabs are displayed: Page, CompassCDS, and System. Selecting one of these tabs and then clicking on a variable in the associated list, adds that variable to the report.

The Page tab enables a user to print the page number, the total page numbers, and the report-guide variable, which associates a unique number with each report.

The CompassCDS tab enables a user to print the CompassCDS variables. It is also possible to print the Archive number of the chromatogram, by adding the variable $ARCHIVERSION.

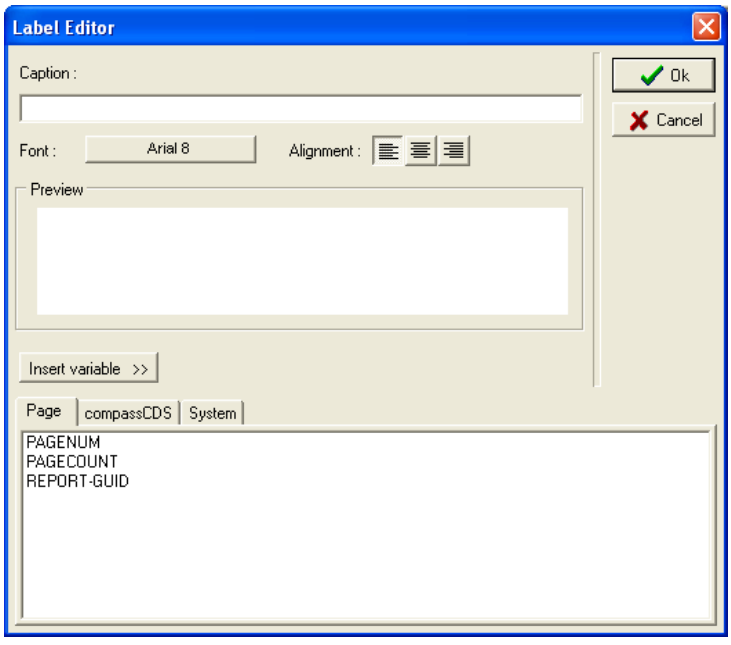
The System tab enables a user to print system variables such as the printing date and time, the computer's name, and the OS version.

For example, if a user types text such as '*The name of the chromatogram is*' and then selects the variable CHROMATONAME, the name of the chromatogram will be printed after the words the user typed.

Label Object

This object enables a user to create and to insert a label, for example, title of the report. A user can define the caption font style, size, and color.

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



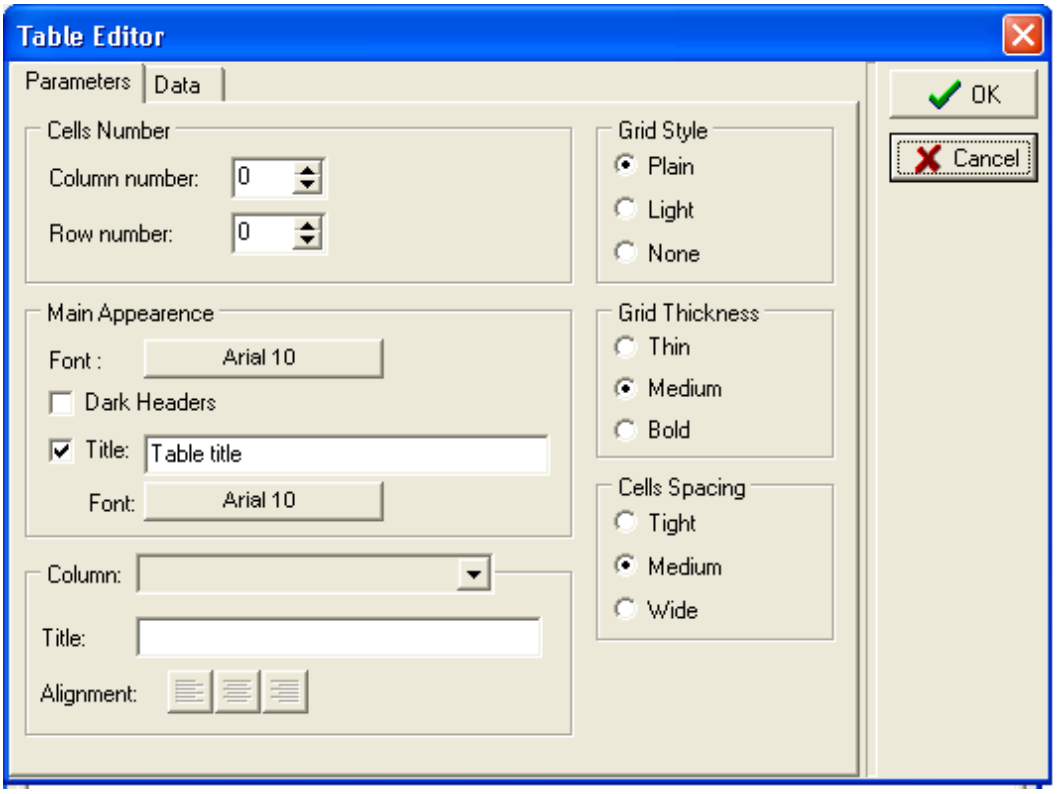
In the Caption area, enter the words to be displayed, e.g., 'Analysis report'. A user can also insert a variable (as with the text object) with the Insert variable>> button.

Clicking on the Font button modifies the font style, size, and color. The buttons enable a user to modify the text alignment.

Table Object

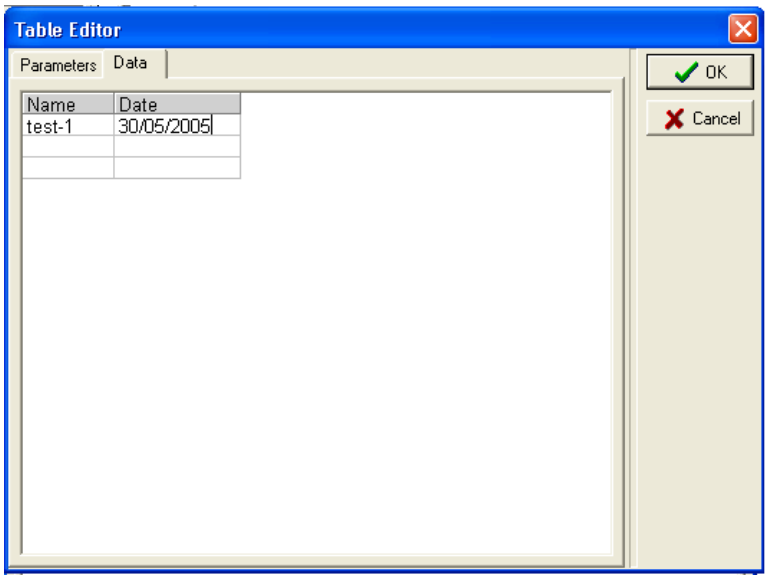
Adds a table.

A user can select the PROPERTIES option in the popup menu to configure this object once it has been selected. The following window will appear:



A user can select the table size and customize its display (grid style, thickness, cell spacing, and main appearance) by clicking on the Table Editor Parameters tab. A user can also name the columns of the table.

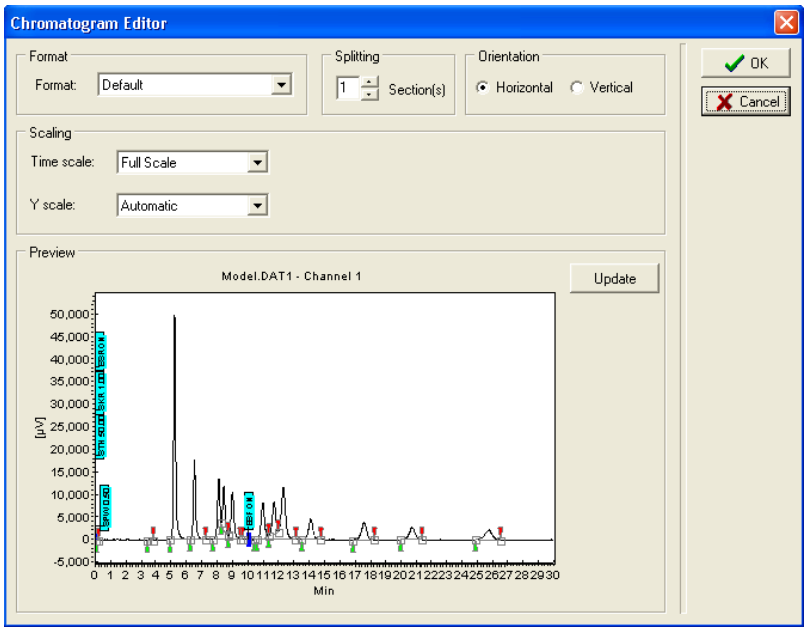
Select the Data tab to add data into the table.



Chromatogram Object

This object enables a user to add a chromatogram to the report.
In the pop-up menu select PROPERTIES to configure the object.

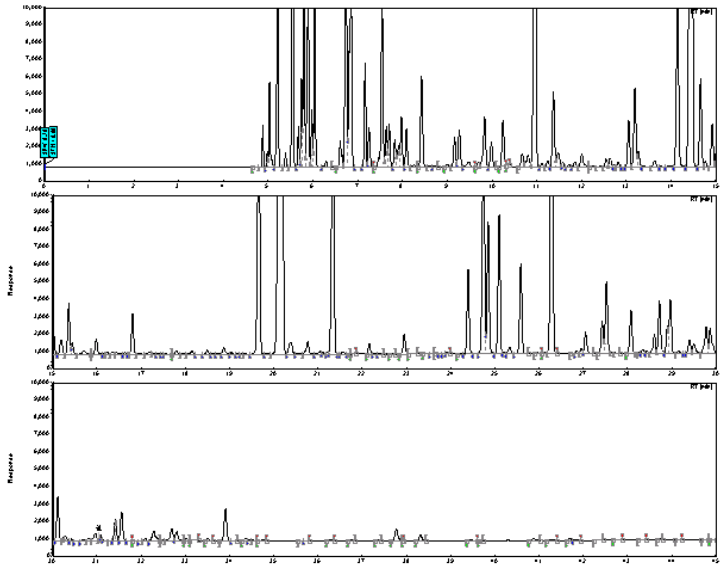
The following window appears:



In the Format area, choose the chromatogram format configured in CompassCDS (in the format section of the method). The chromatogram can be opened in CompassCDS with one format and printed with another format.

In the Splitting area, choose the number of sections in which to split the chromatogram.

Example: 3 sections



In the Orientation area a user can select whether the chromatograms are to be printed horizontally or vertically.

In the Scaling area, a user can modify both the time scale and the amplitude scale.

Time Scale: The time range represents the limits of the chromatogram X axis.

Full scale: The chromatogram is printed in maximum scale (from zero to the end of the acquisition).

Custom: Select this option to specify manual limits to the chromatogram. When this option is selected, some edit boxes appear:

Peak # or Named peak: Select this option to print a peak only. User has to choose which peak to print by choosing either its name or its index.

Working scale: Select this option to print the chromatogram in the scale defined in CompassCDS. This scale can be defined in the Quick Start windows (or in the acquisition area of the method), or after the acquisition in the working scale.

Y Scale: This amplitude range is the limit of the chromatogram ordinates.

Automatic: The chromatogram is printed with the acquisition scale.

Custom: Select this option to manually specify the limits of the chromatogram amplitude. When this option is selected, the following edit boxes appear:

% highest peak: Select this option to scale the chromatogram according to the height of one of the peaks (defined by its relative height). For example, if a user choose to plot the chromatogram up to 200% of the second highest peak, the maximum Y value will be twice the height of the second highest peak.

Named peak: Select this option to scale the chromatogram according to the height of one of the named peaks. For example if a user choose to plot the chromatogram up to 200% of the peak Butane, the maximum Y value will be twice the height of the peak Butane.

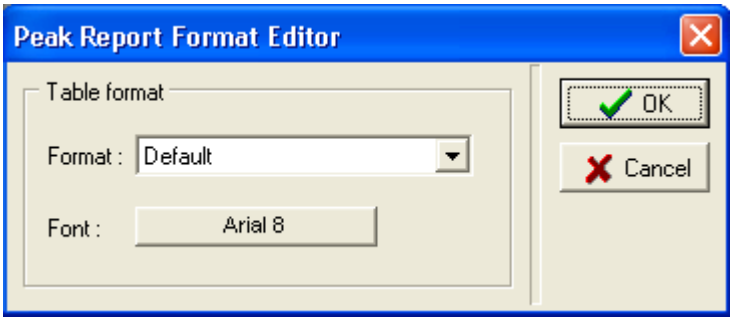
A chromatogram preview allows a user to view the chromatogram as it will be printed, according to the selected options. Clicking on the Update button takes into account the options chosen in the fields of the chromatogram properties.

Peak Results Object

This object enables a user to insert the peak results. A user can customize the table (font style, size, and color) and select a specific format.

The Peak Report contains all the peaks integrated into the chromatogram. (Select RESULTS / PEAK REPORT in the browser to display the Peak Report in CompassCDS Chromatography Data System.)

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



The Peak Table can be printed with a specific format. In CompassCDS it is possible to define formats in the method or in the peak table properties (see CompassCDS User Guide). One of these formats can be applied to the printing.

The Peak Table formats are saved with a specific name and a comment in CompassCDS. Select the corresponding name in the Format dropdown list, and the comment will appear.

In the Peak Results properties a user can modify the appearance of the table using the Font button.

Note that the printed table can have a different format from the one displayed in CompassCDS (Results).

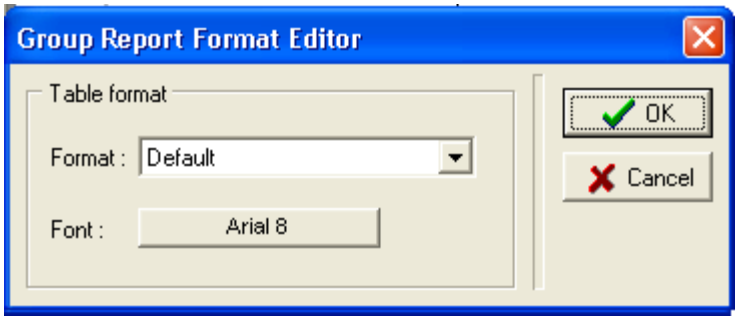
Group Results Object

This object enables a user to insert the group results. A user can customize the table (font style, size, and color) and select a specific format.

The Group Report is the table containing all the groups defined in the chromatogram. Select RESULTS/GROUP REPORT in the browser to display the Group Report in CompassCDS.

The group table can be configured in the same way as the peak table.

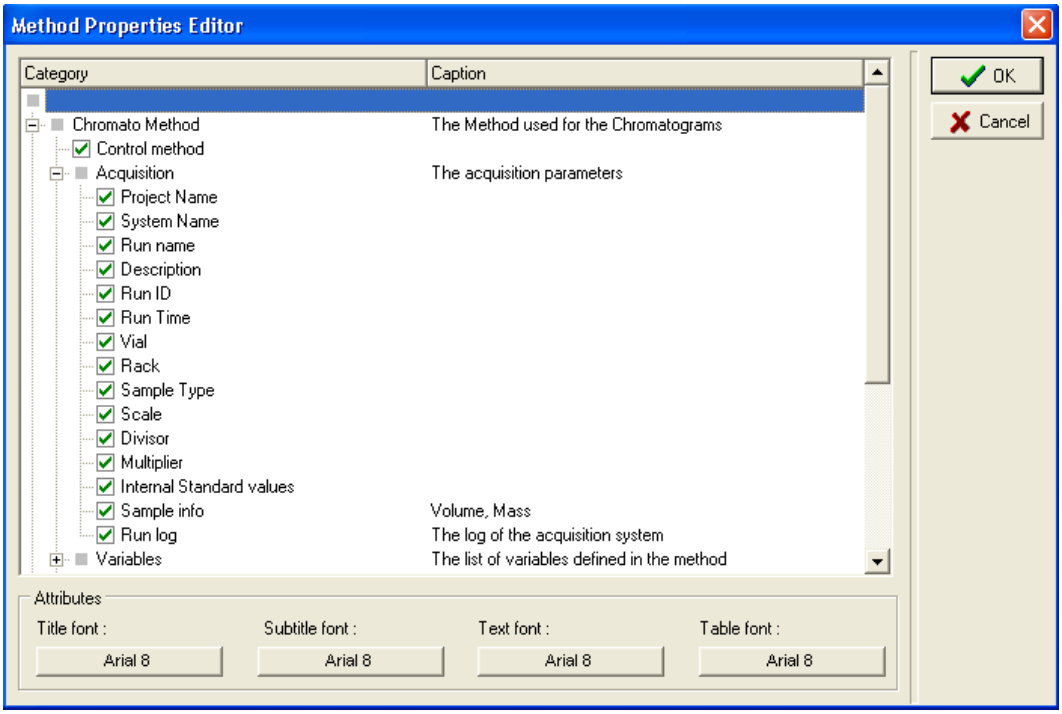
In the pop-up menu select PROPERTIES to configure the object. The following window appears:



Method Object

This object enables a user to insert the method.

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



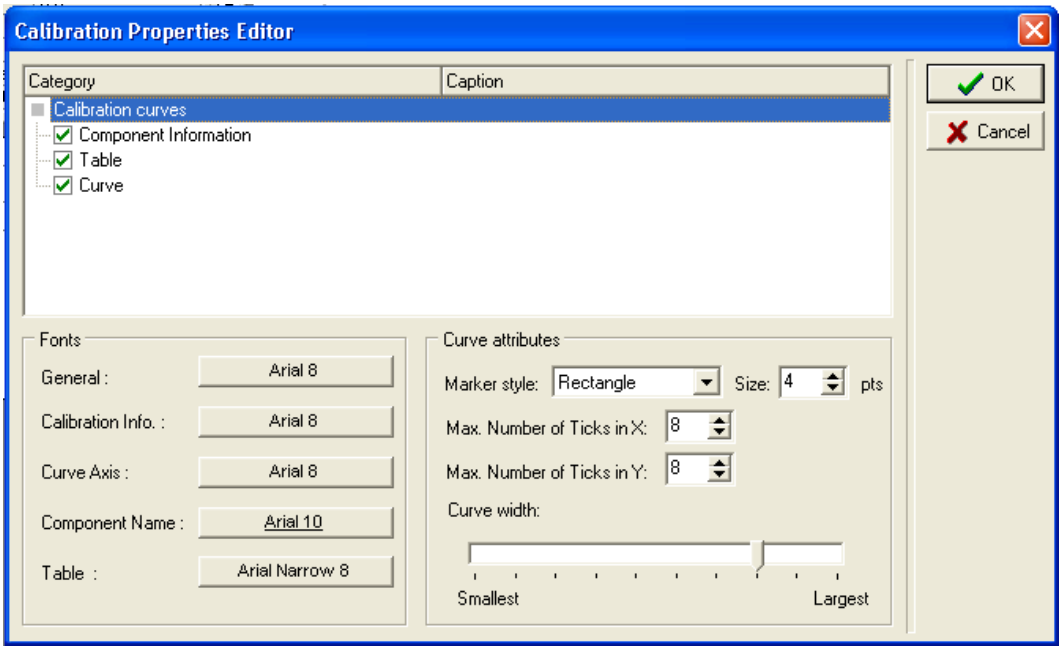
A user can check the sections of the method to print and uncheck the ones that are not to be printed.

NOTE: The acquisition parameters printed are the ones entered at the acquisition time. If the chromatogram has been reprocessed with different parameters, then they will not be printed in this part. The latest ones are in the global variables available in a text or a label object.

Calibration Report Object

This object enables a user to print the Calibration Report.

In the pop-up menu select PROPERTIES to configure the object. The following window appears:



A user can check the calibration parameters that are to be printed and uncheck the parameters that are not required to be printed.

- Component information: prints the mathematical model, the calibration curve equations, the regression coefficients, the weighting, and forcing through (0,0).
- Table: prints the calibration point tables displayed in the 'Calibration' tab in CompassCDS, the list of the calibration points, their origin, the acquisition date, the name of the user that added the point, etc.
- Curve: Prints the calibration curves.

In the Fonts area, a user can select the fonts for the different areas of the Calibration object.

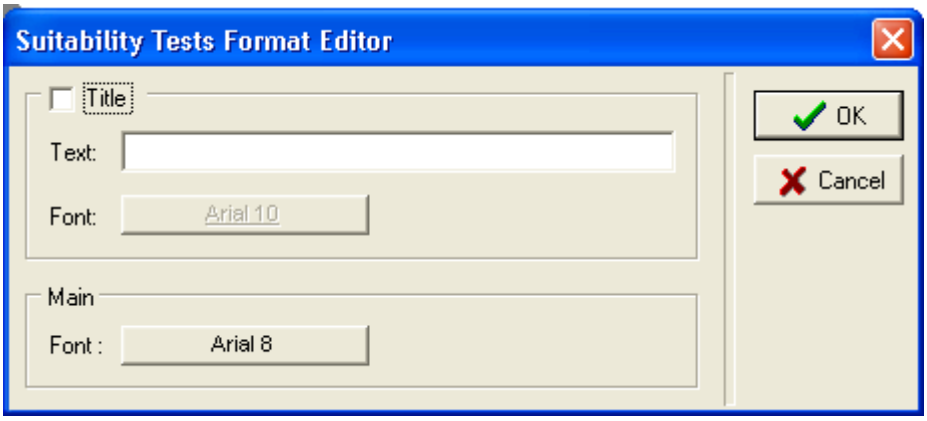
- General: name of the calibration curve.
- Calibration info: equation, correlation factors.
- Curve axis: curve axis names, graduations.
- Component name: name of the component.
- Table: font used for all table fields.

In the 'Curve attributes' field a user can configure the style of the printed calibration curve displaying: type and size of the marker style, number of ticks in X and Y axis and location of the calibration curve on the page using the curve width bar. The curve is always placed on the right side of the page.

Suitability Tests Object

This object enables a user to print the results of the suitability tests.
The suitability tests are defined in the Method.

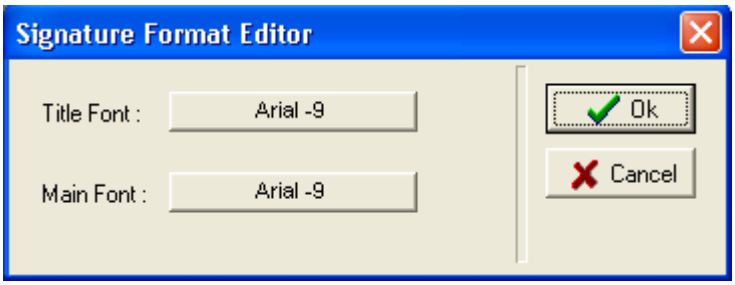
In the pop-up menu select PROPERTIES to configure the object. The following window appears:



A user can define a Suitability Tests title in the dedicated field (check the title box) and define the font style, size, and color.

Electronic Signature Object

This object enables a user to print the electronic signature.
In the pop-up menu select PROPERTIES to configure the object. The following window appears:



A user can define the font displayed in the table: Title Font for the title, Main Font for the content of the table.

Default Reports

Eight default report styles are available for use and can be found in the CompassCDS/data folder.

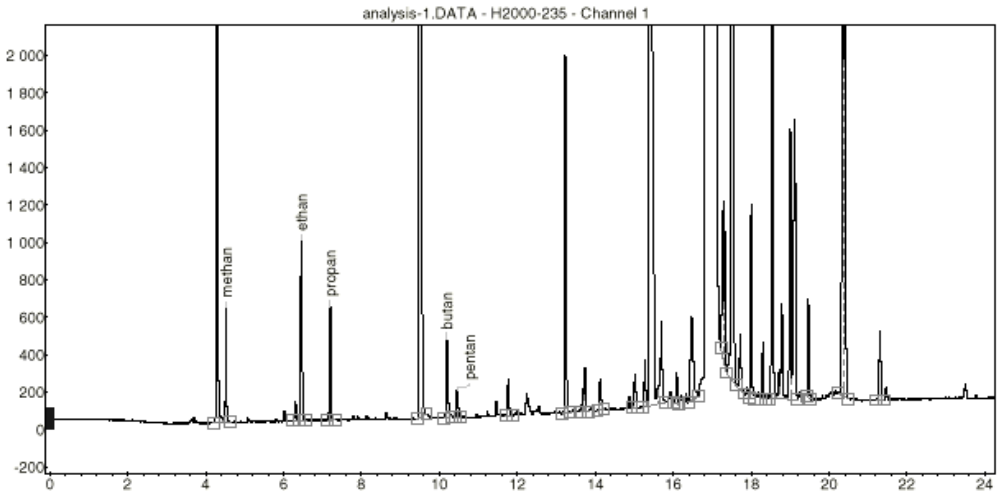
A user will need to copy these into the Group subfolder where they are required for use.

Default_standard.STYL:

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 12:04:01
Printed : 26/04/01 12:11:07



Peak results :

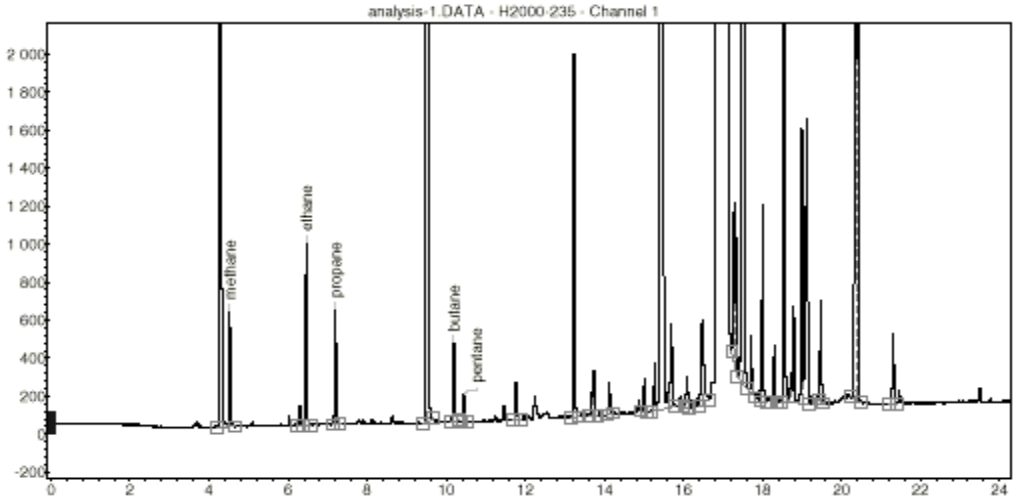
Index	Name	Time	Quantity	Area	Area
		[min]	[mass ratio]	[µV.min]	[%]
2	methan	4.52	0.00	19.3	0.034
4	ethan	6.46	0.00	37.6	0.066
5	propan	7.20	0.00	24.8	0.044
7	butan	10.19	0.00	21.7	0.038
8	pentan	10.46	0.00	7.0	0.012
Total			0.00	56793.2	100.000

Default_group_standard.STYL

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 17:15:44
Printed : 26/04/01 17:16:59



Peak results :

Index	Name	Time	Quantity	Area	Area
		[min]	[g/l]	[µV.min]	[%]
2	methane	4.52	5.90	19.3	0.034
4	ethane	6.46	0.00	37.6	0.066
5	propane	7.20	10.23	24.8	0.044
7	butane	10.19	0.00	21.7	0.038
8	pentane	10.46	0.00	7.0	0.012
Total			16.13	56793.2	100.000

Group results :

Index	Name	Area	Area
		[µV.min]	[%]
1	group1	55349.4	97.458
2	group2	1333.4	2.348
Total		56682.7	99.806

Default calibration.STYL

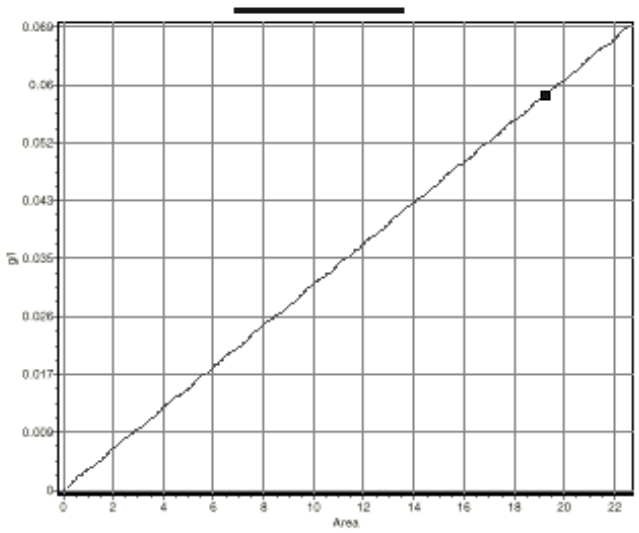
Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 16:03:03
Printed : 26/04/01 16:11:13

Calibration Report :
File : alkanes

Component : methane
Polynom : y = b x + a
a = 0
b = 3.06394E-003
Correlation Coef. : -1.0000
Weighting : None
Force zero : Yes



Calibration table : methane

#	Used	Name	Area	gl	Chromatogram	Date	gl (residual)	Res %	time [min]	Level	Username
1	1	Point 1	18.26	0.05	analysis-1 - 1	26/04/01 15:47:57	0.06	0.00	4.62	1	sv

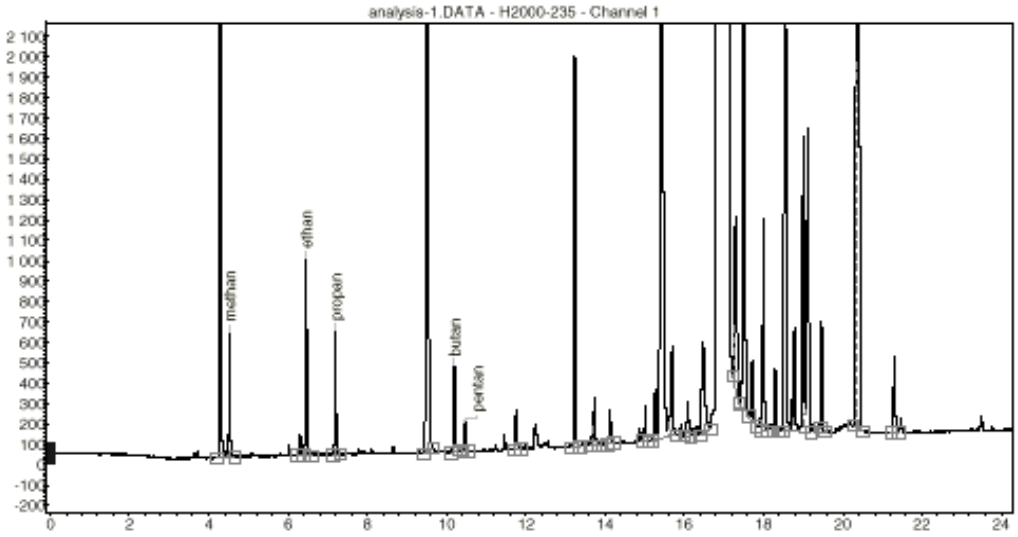
Component : propane
Polynom : y = b x + a
a = 0

Default suitability.STYL

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 14:00:24
Printed : 26/04/01 14:00:53



Peak results :

Index	Name	Time	Quantity	Area	Area
		[min]	[mass ratio]	[µV.min]	[%]
2	methan	4.52	0.00	19.3	0.034
4	ethan	6.46	0.31	37.6	0.066
5	propan	7.20	0.00	24.8	0.044
7	butan	10.19	0.18	21.7	0.038
8	pentan	10.46	0.06	7.0	0.012
Total			12.29	56793.2	100.000

Suitability Results :

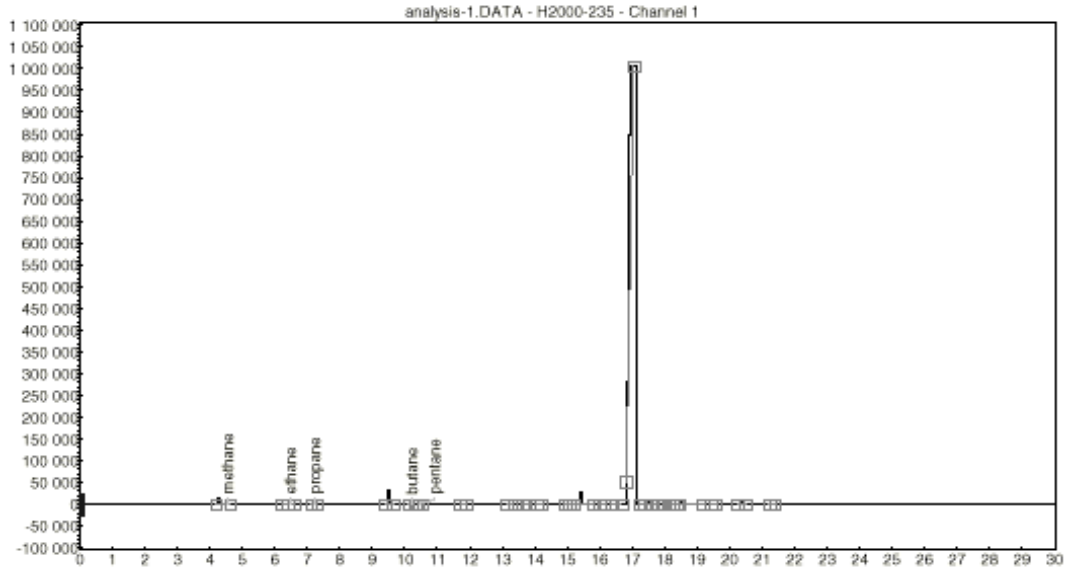
For Peakmethan : if test *AREAP = 10.00 fails then report only: Failed! (production problem)

Default_method.STYL

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 16:31:53
Printed : 26/04/01 16:51:40



Results :

Index	Name	Time	Quantity	Area	Area
		[min]	[g/l]	[µV.min]	[%]
2	methane	4.52	5.90	19.3	0.034
4	ethane	6.46	0.00	37.6	0.066
5	propane	7.20	10.23	24.8	0.044
7	butane	10.19	0.00	21.7	0.038
8	pentane	10.46	0.00	7.0	0.012
Total			16.13	56793.2	100.000

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 17:24:04
Printed : 26/04/01 17:24:25

CHROMATOGRAM METHOD REPORT :

Acquisition :

Run Time : 30.00
Vial : 0
Rack : 0
Divisor factor : 1.00
Multiplier factor : 100.00
Analysis : Sample
Injection volume : 1.00 µl
Injection amount : 12 067.30

Preprocessing :

Blank Subtract :

File:
N.A.

Integration Method :

Reduce Noise : Yes
Spike Parameter : 1
Use Relative Threshold : Yes

Integration Events :

Active	Time	Event	On	Value
Yes	0.00	Set Peak Width		0.2
Yes	0.00	Set Threshold		4

Manual actions :

Manual integration action count : 0

Peak Identification table :

Peak Name	RT [min]	Abs.Window[min]	Window %	Ref ?	Mode	Group
methane	4.53	0.20	0.20		Nearest	
ethane	6.47	0.20	0.20		Nearest	
propane	7.22	0.20	0.20	X	Nearest	
butane	10.21	0.20	0.20		Nearest	
pentane	10.44	0.20	0.20		Nearest	

Resolve with references : Yes

Group Identification table :

Group Name	Group type	Parameters
group1	Calibration group	1 range(s)
group2	Calibration group	1 range(s)

Calibration Method :

Method type : External Standard
Response : Area
Standard Unit : g/l
Calibration curve file name : alkanes

Factors : Curve
Subtract internal standard mass
Response unit : Curve

Unknown mode : Response Factor
Factor value : 0.025
Internal Standard

Componer	Model	Weighting	Poly Order	(0,0) ?	Level 1
methane	Polynomia	N/A	1	X	5.90

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 16:31:53
Printed : 26/04/01 16:51:40

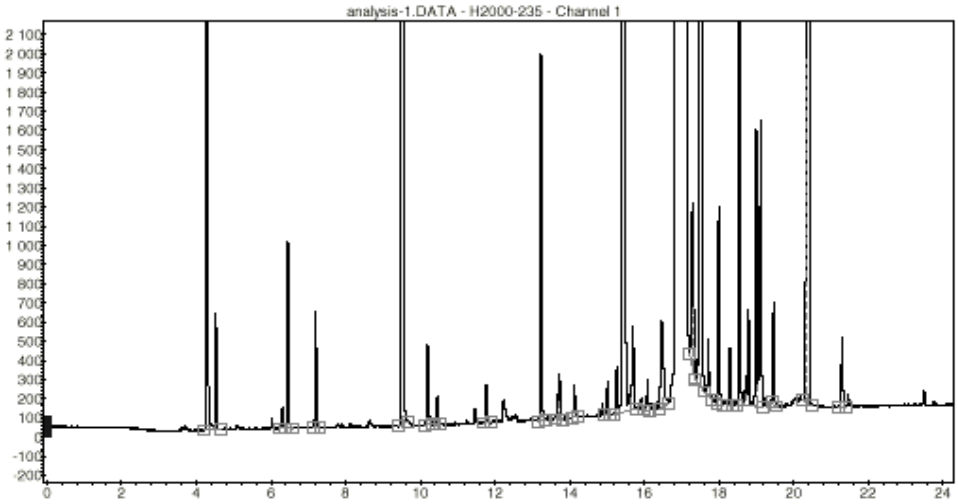
Componer	Model	Weighting	Poly Order	(0.0) ?	Level 1
propane	Polynomia	N/A	1	X	10.23

Default_group_method

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 17:24:04
Printed : 26/04/01 17:24:25



Peak results :

Index	Name	Time	Quantity	Area	Area
		[min]	[g/l]	[µV.min]	[%]
2	methane	4.52	5.90	19.3	0.034
4	ethane	6.46	0.00	37.6	0.066
5	propane	7.20	0.00	24.8	0.044
7	butane	10.19	0.00	21.7	0.038
8	pentane	10.46	0.00	7.0	0.012
Total			5.90	56793.2	100.000

Group results :

Index	Name	Area	Area
		[µV.min]	[%]
1	group1	55349.4	97.458
2	group2	1333.4	2.348
Total		56682.7	99.806

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 17:24:04
Printed : 26/04/01 17:24:25

CHROMATOGRAM METHOD REPORT :

Acquisition :

Run Time : 30.00
Vial : 0
Rack : 0
Divisor factor : 1.00
Multipliplier factor : 100.00
Analysis : Sample
Injection volume : 1.00 µl
Injection amount : 12 067.30

Preprocessing :

Blank Subtract :

File:
N.A.

Integration Method :

Reduce Noise : Yes
Spike Parameter : 1
Use Relative Threshold : Yes

Integration Events :

Active	Time	Event	On	Value
Yes	0.00	Set Peak Width		0.2
Yes	0.00	Set Threshold		4

Manual actions :

Manual integration action count : 0

Peak Identification table :

Peak Name	RT [min]	Abs.Window[min]	Window %	Ref ?	Mode	Group
methane	4.53	0.20	0.20		Nearest	
ethane	6.47	0.20	0.20		Nearest	
propane	7.22	0.20	0.20	X	Nearest	
butane	10.21	0.20	0.20		Nearest	
pentane	10.44	0.20	0.20		Nearest	

Resolve with references : Yes

Group Identification table :

Group Name	Group type	Parameters
group1	Calibration group	1 range(s)
group2	Calibration group	1 range(s)

Calibration Method :

Method type : External Standard
Response : Area
Standard Unit : g/l
Calibration curve file name : alkanes

Factors : Curve
Subtract internal standard mass
Response unit : Curve

Chromatogram : analysis-1_channel1

System : GC_59
Method : sample analysis
User : sv

Acquired : 05/12/00 12:00:50
Processed : 26/04/01 17:24:04
Printed : 26/04/01 17:24:25

Unknown mode : Response Factor
Factor value : 0.025
Internal Standard

Componer	Model	Weighting	Poly Order	(0,0) ?	Level 1
methane	Polynomia	N/A	1	X	5.90

CompassCDS
Enhanced Chromatogram Report
Plug-in User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2018
Publication Number BR501579
Revision E

Contents

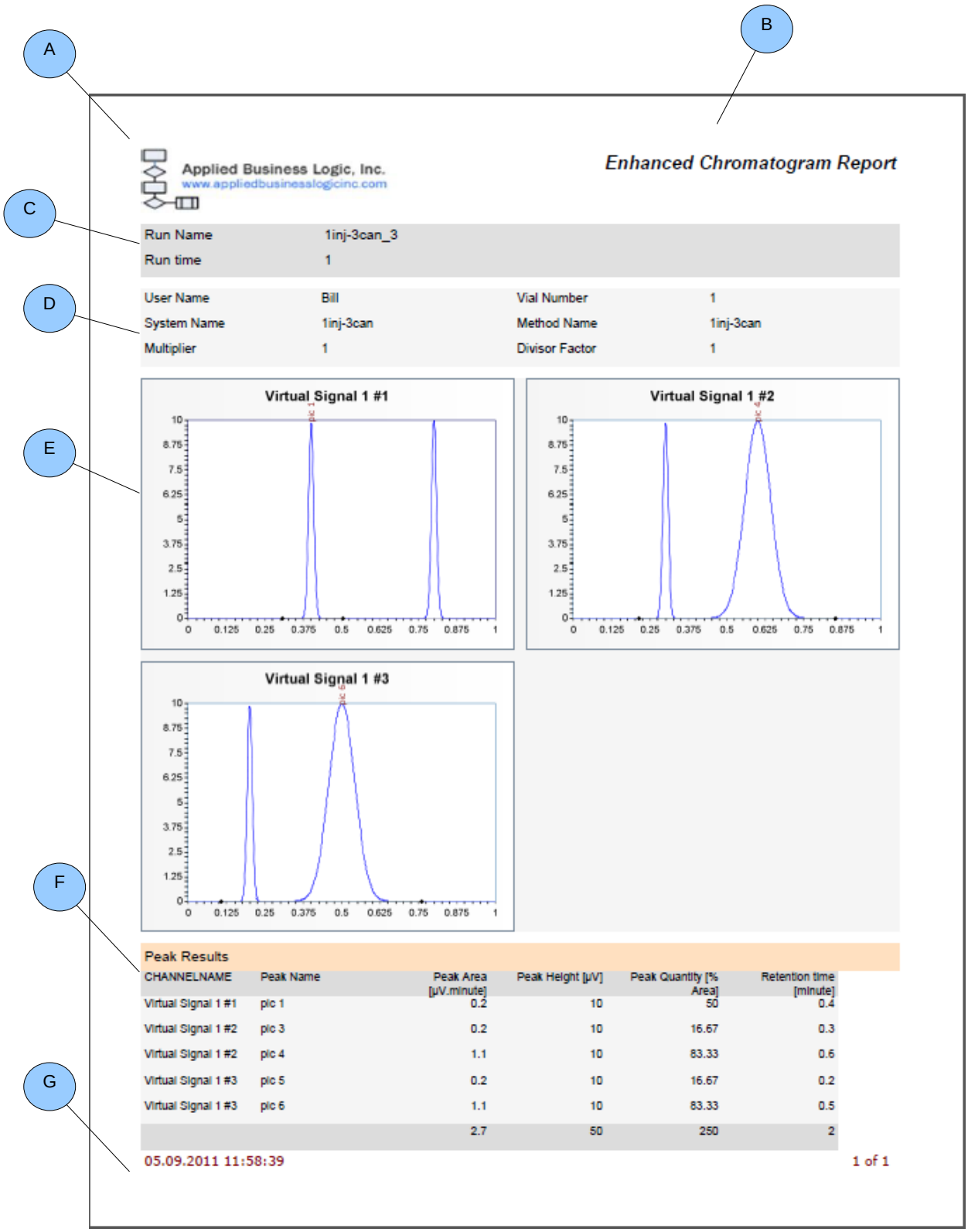
Introduction....3
The Enhanced Chromatogram Report at a Glance....4
Software Prerequisites....5
Installing the Enhanced Chromatogram Report Plug-in....5
Configuring the Enhanced Chromatogram Report Plug-in....6
  Configuring the General Settings....6
  Configuring the Headers....7
  Configuring Charts....7
  Configuring Results Display....8
  Configuration Defaults....9
Running the CompassCDS Enhanced Chromatogram Report Plug-in....9
  Logging....9

Introduction

The Enhanced Chromatogram Reporter produces a customizable graphical / tabular view of all data for a given run. The report displays a chromatogram for all channels (1 to 4), along with a table of results for each peak. The report is configured as a CompassCDS post-run plug-in but can also be run in Direct Mode via the toolbar menu Plug-ins option. The process renders the report in the industry standard PDF format which is read using Adobe Reader.

This document describes the advanced features and configuration of this report.

The Enhanced Chromatogram Report at a Glance


A
B
C
D
E
F
G
Applied Business Logic, Inc.
www.appliedbusinesslogicinc.com
Enhanced Chromatogram Report
Run Name 1inj-3can_3
Run time 1
User Name Bill
Vial Number 1
System Name 1inj-3can
Method Name 1inj-3can
Multiplier 1
Divisor Factor 1
Virtual Signal 1 #1
Virtual Signal 1 #2
Virtual Signal 1 #3
Peak Results
CHANNELNAME Peak Name Peak Area [µV.minute] Peak Height [µV] Peak Quantity [% Area] Retention time [minute]
Virtual Signal 1 #1 pic 1 0.2 10 50 0.4
Virtual Signal 1 #2 pic 3 0.2 10 16.67 0.3
Virtual Signal 1 #2 pic 4 1.1 10 83.33 0.6
Virtual Signal 1 #3 pic 5 0.2 10 16.67 0.2
Virtual Signal 1 #3 pic 6 1.1 10 83.33 0.5
2.7 50 250 2
05.09.2011 11:58:39
1 of 1

A. Custom header graphics are interchangeable and users can insert a company logo onto the report. This is done by simply re-naming the “logo.jpg” that is located in the C:\Program Files\Scion\Enhanced Chromatogram Report\ folder and replacing it with the desired logo named ‘logo.jpg’. The logo will be displayed in the upper-right corner of the report (300X100 px graphic).

B. Report Name can be configured via configuration dialog.

C. Page Header appears at the top of each page and can be configured using any CompassCDS Global variables.

D. Report header appears at the top of the first page and can be configured using any CompassCDS Global variables.

E. Graphical chromatograms shown for up to four detector channels.

F. The Peak Results table is displayed below the chromatogram. The table can be separated by channel, or all of the results combined into a single table. Group Results are supported in the same way. Group table(s) appear after Peak Result tables. Peak and Group table columns are configured via the configuration dialog.

G. The report footer shows time/date (in localized format), and page number.

Software Prerequisites

- The plug-in requires .NET Framework 3.5. The installer will prompt the user to install if it has not been installed. This application can be found in the Tools folder on the CompassCDS DVD or downloaded from https://www.microsoft.com/en-us/download/details.aspx?id=21
- Microsoft Report Viewer Redistributable 2008: https://www.microsoft.com/en-us/download/details.aspx?id=6576
- Adobe Reader, used to read PDF files. This application can be found on the CompassCDS DVD or downloaded and installed from: https://get.adobe.com/de/reader/?promoid=BUIGO
- CompassCDS Version 4.0 or higher.

Installing the Enhanced Chromatogram Report Plug-in

1. Using Windows Add/Remove Programs, uninstall any previously installed version of the Enhanced Chromatogram Report Plug-in.

2. Run the attached Setup.exe file and follow the prompts to complete the install.

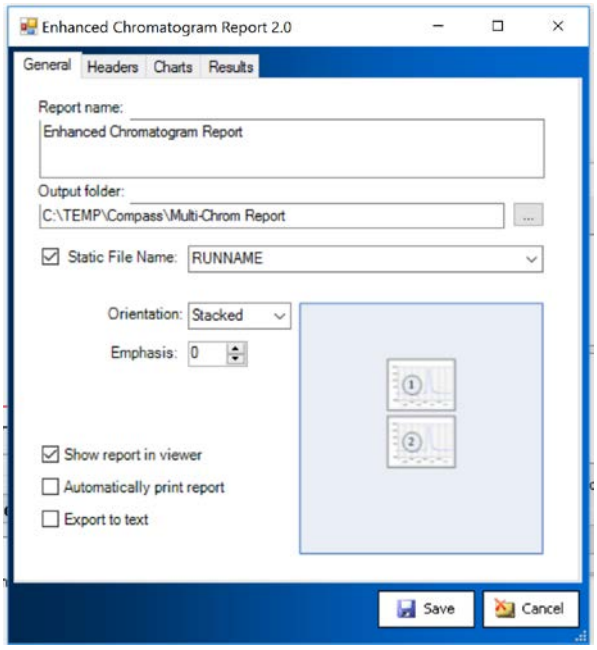
Configuring the Enhanced Chromatogram Report Plug-in

1. The CompassCDS Enhanced Chromatogram Report is configured as a post-run plug-in within the CompassCDS method. Click the post-processing section of the method, then click Add and follow the steps to add the plug-in.

NOTE: If the plug-in does not appear in the CompassCDS list for post-run plug-ins, double click the included MultiChannelChromatogramReport.reg file to manually register the plug-in. Restart CompassCDS.

2. Once the plug-in has been added to the method, it must be configured. Click the Configure button on the CompassCDS dialog.

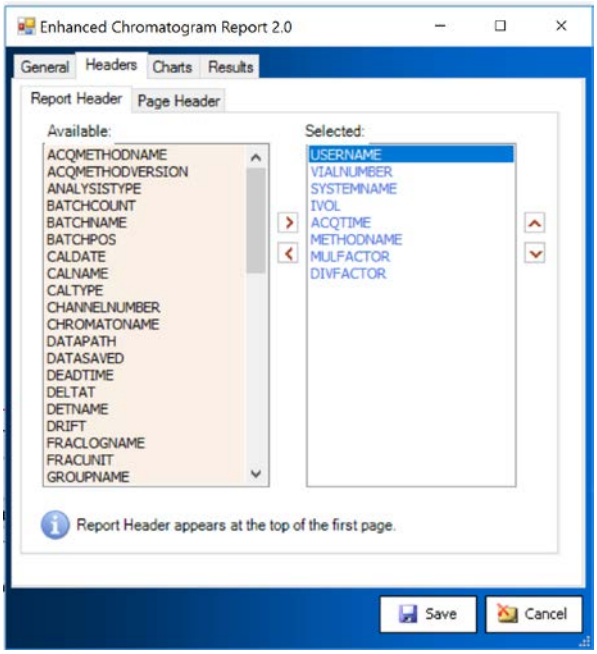
Configuring the General Settings



1. Specify the Report Name to appear in the Report Header
2. Select the output folder where all reports will be written.
3. Select the option to use a static file name based on any CompassCDS Global Variable. If left unchecked, the program creates a random (unique) file name.
4. Control the orientation of the chromatograms appearing on the report (Stacked or Standard).
5. Set the Emphasis on a particular channel to make this chromatogram larger than the rest.
6. Check to show the report in the Adobe Reader viewer after the PDF file has been created.
7. Check to enable silent printing of the report to the default printer without showing the chromatogram in the viewer.

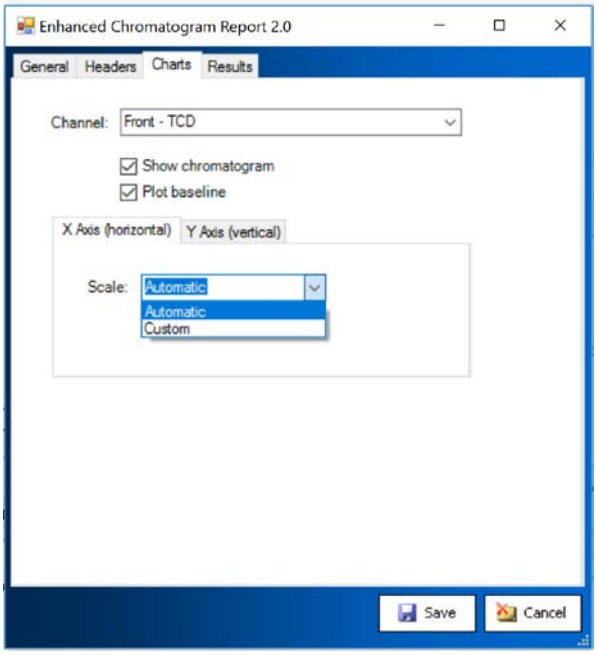
Configuring the Headers

The CompassCDS Enhanced Chromatogram Report has two header sections; Report Header and Page Header. Each is configured separately.



1. The Report Header is displayed only at the top of the first page.
2. The Page Header is displayed at the top of each page.
3. Users may configure each header section by selecting from a list of CompassCDS variables that can include custom variables.

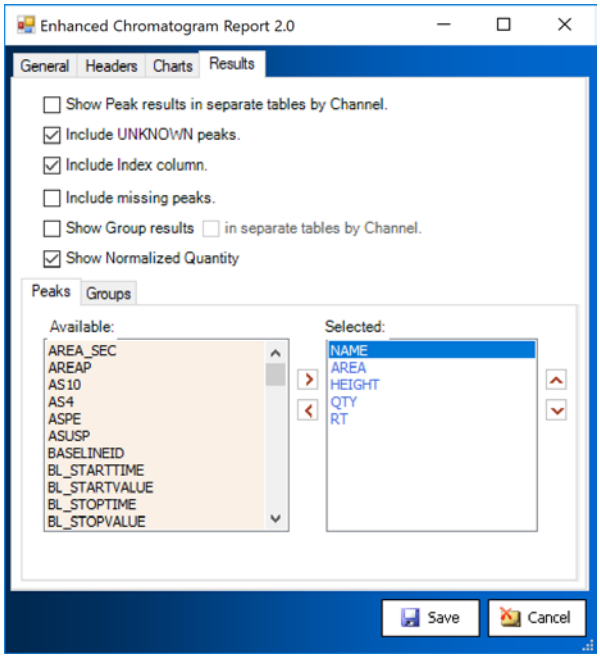
Configuring Charts



Select the channel from the Channel dropdown. For each channel, the following changes can be made:

- Click Show chromatogram to have the selected channel appear on the report.
- Select Plot Baseline to have the baseline plotted in the graph.
- Select Include UNKNOWN peaks to include the UNKNOWN summary row in the tabular output.
- The scale for both X and Y axis can be configured independently for each channel. Selecting Automatic (default) allows the charting program render a best-fit scale. Choosing Custom allows the user to specify a From and To value for a given axis.

Configuring Results Display



1. The report can display PEAK results in separate tables (per channel), or combine all results into a single table.
2. The report can include or exclude UNKNOWN peaks.
3. Include/exclude the index (row count) column in the tabular output.
4. Users can choose to include missing peaks, where peaks specified in the method were not detected in the run. Results values for these peaks will be zero.
5. The report can show GROUP results in separate tables (per channel), or combine all GROUP results into a single table.
6. The report can show normalized results for the quantity variable.
7. Users can select tabular report columns for PEAKS by selecting from available CompassCDS variables/custom variables at the peak level.
8. Users can select tabular report columns for GROUPS by picking from available CompassCDS variables/custom variables at the group level.

Configuration Defaults

When the CompassCDS Enhanced Chromatogram Report is first configured in the post-run section of the method (or data file), the defaults for all settings are managed via the ecr.config file. Special care must be taken when editing this file. Examples below:

- Default the report name:
  <Setting Name="DEFAULT_REPORTNAME" Value="Enhanced Chromatogram Report" />
- Default columns for peak results table (comma-separated list):
  <Setting Name="DEFAULT_PEAKVARIABLES" Value="NAME,AREA,HEIGHT,QTY,RT" />

Running the CompassCDS Enhanced Chromatogram Report Plug-in

Post Run: Once configured, the CompassCDS Enhanced Chromatogram Report plug-in runs automatically after each run. During this process, raw data is gathered from CompassCDS via the API and then transformed into each chart. The results table is also built using CompassCDS API calls. The report is rendered into .PDF format and can be read using the Adobe Reader application. Depending on the size of the data file, this process can take as long as 30 seconds to complete.

Direct Mode: The CompassCDS Enhanced Chromatogram Report plug-in can also be launched from the main CompassCDS toolbar. The “Plug-in menu item” on the toolbar launches the report. Note: a CompassCDS Chromatogram method file MUST be loaded into the Data view for this to work.

Logging

During report execution, messages are written to log.txt file found in the logged-in users’ Application Data folder (C:\Documents and Settings\User1\Application Data). These include tracing/status messages along with error messages.

CompassCDS
Arithmetic Functions Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501487
Revision D

Contents

Software Presentation....3
Overview....3
Installation....3
Application Details....4
How to Use the Arithmetic Functions Plug-in....4
Operand Selection....5
Operator Selection....6
Calculation Parameters....7
Addition....7
Subtraction....8
Multiplication....8
Division....8
Weighting Sum....8
Generation of a Chromatogram Usable in CompassCDS....10
Saving the Generated Chromatogram....10
Loading a Virtual Chromatogram in CompassCDS....10
Returning to CompassCDS without Generating a Virtual Chromatogram....11

Software Presentation

This document describes the Arithmetic functions Plug-in for CompassCDS.

Overview

The Arithmetic functions Plug-in enables mathematical operations between either chromatograms or chromatograms and real numbers.

It operates like a calculator with two operands, one operator and one result.

Each operand can be either selected among chromatograms loaded in CompassCDS or in the chromatograms storage directory. A numerical zone is also available to execute an operation between a chromatogram and a real number.

Different operators are available and these include: Addition, Multiplication, Subtraction, Division, and Weighted sum.

Once the operands have been selected, the operation is validated by clicking on the operator button. The result is then displayed in the bottom left of the screen.

Installation

Insert the CompassCDS media in the CD/DVD drive.

Check the following files are present in the C:\CompassCDS\client folder.

- AX_arithmetic.dll
- Diamirdefaultmethod.meth: It allows the user to save calculated chromatograms with this default CompassCDS method

Select the AX_Arithmetic.dll file and drag and drop it on the C:\CompassCDS\client \TRegSvr.exe to merge the file with the registry.

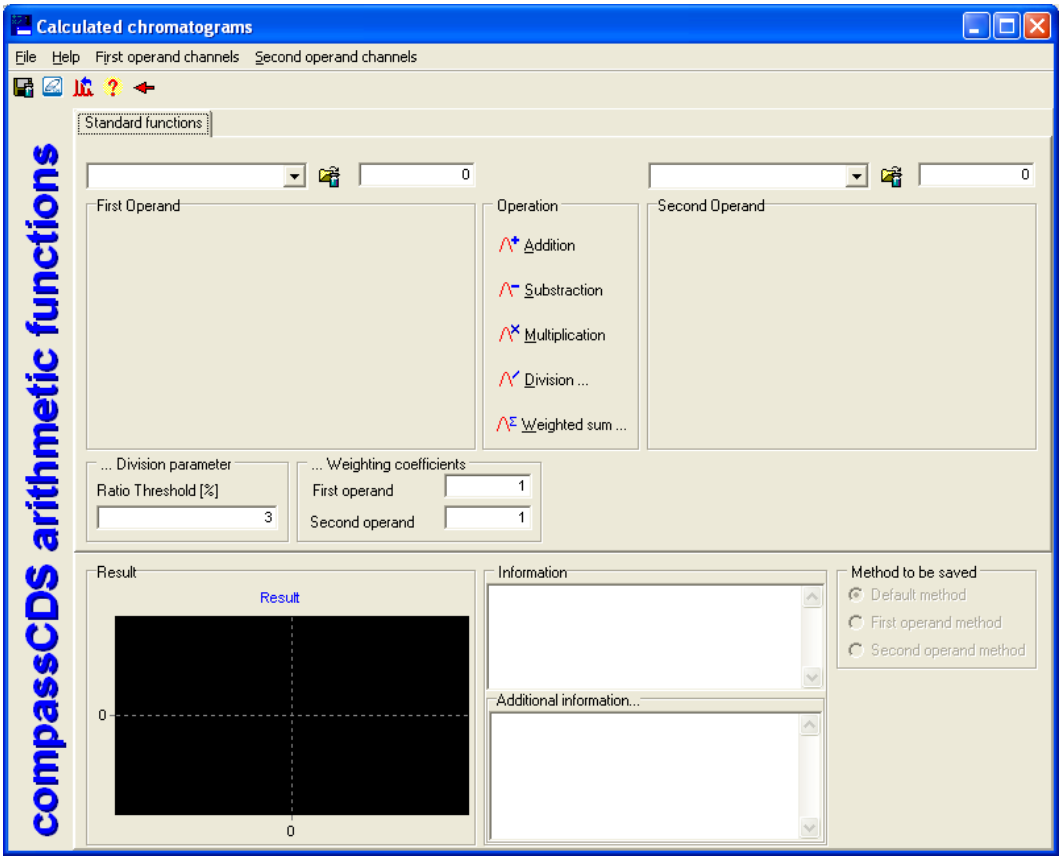
Start CompassCDS, check that the icon allows to access the “Arithmetic functions” plug-in.

Application Details

How to Use the Arithmetic Functions Plug-in

In CompassCDS, open the Arithmetic plug-in by selecting the

icon. The following screen is displayed:



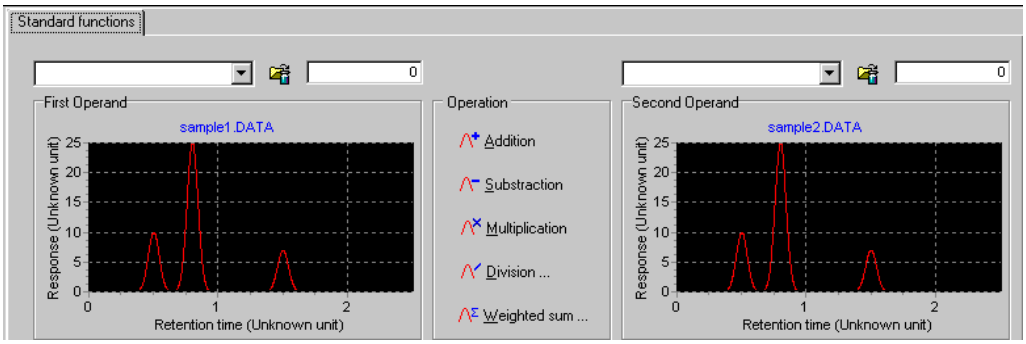
The main screen is divided into two parts:

The first part enables a user to select the chromatogram(s) on which the calculations (called Operand) is performed, and the type of calculation (by choosing Operation) which will define the function. A second part is dedicated to result viewing.

Icons enable a user to save the virtual chromatogram generated, and open it into the current CompassCDS session.

Operand Selection

The two operands are located in the top left and right of the screen. The operand can be a chromatogram or a real number.

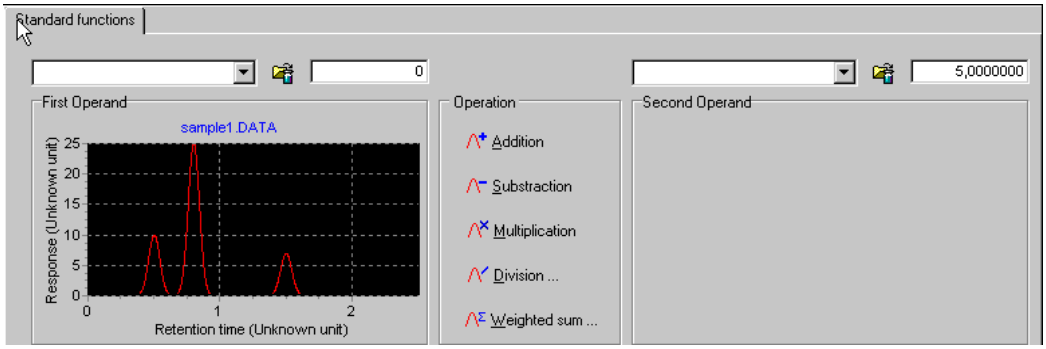


To select Chromatograms, a user has two options:

- If the chromatogram is open in the CompassCDS session, select its name from the scrolling list: .
- If the chromatogram is not open in the CompassCDS session, select the chromatogram via the button.

In an operation between a real number and a chromatogram, the numerical zone next to chromatogram names must be completed. Only one chromatogram and one real number can be entered. The chromatogram is defined in one operand part (left or right) and the real number in the other.

The following screen is displayed:



Operator Selection

Once two operands (2 chromatograms or 1 chromatogram and a real number) have been defined, the user can select the desired operator.

Five operators are available:

Addition

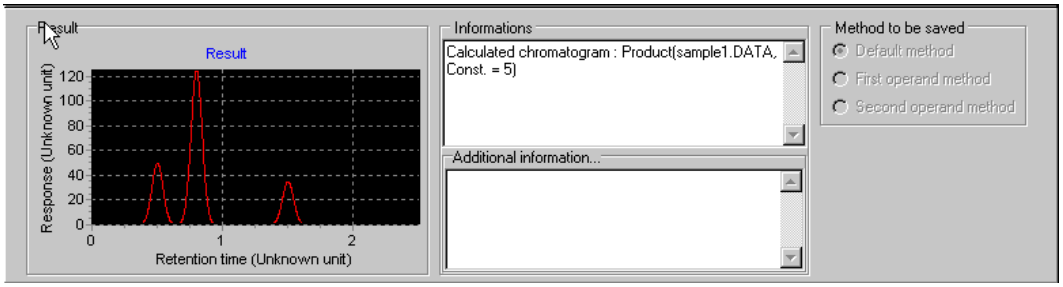
Subtraction

Multiplication

Division

Weighted Sum

As soon as the operator is selected, the result is displayed in the Result part of the screen:



NOTE: The sampling interval and delay time must be identical to process the calculation between chromatograms.

If the retention unit or the response unit is different between chromatograms, a warning is displayed and a user must choose to either ignore the problem and process the calculation, or to cancel it.

If the units are different, the unit saved in the result chromatogram is “Different unit”. If the units are unknown in all the chromatogram parameters, “Unknown unit” will be saved.

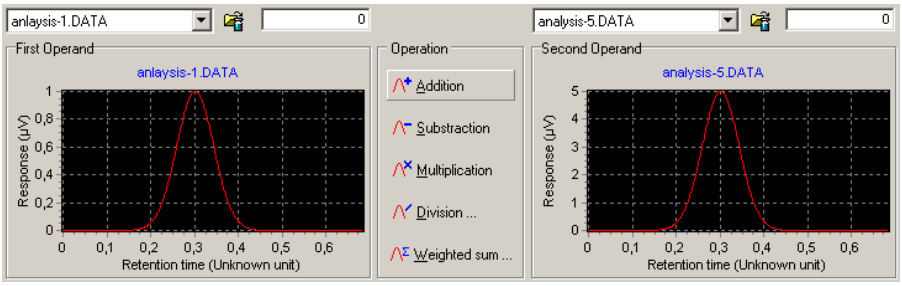
NOTE: If a multi-channel chromatogram is loaded into the Arithmetic Functions Plug-in, a user must select the channel on which calculations are to be performed in the FIRST OPERAND CHANNELS or the SECOND OPERAND CHANNELS menus.

Calculation Parameters

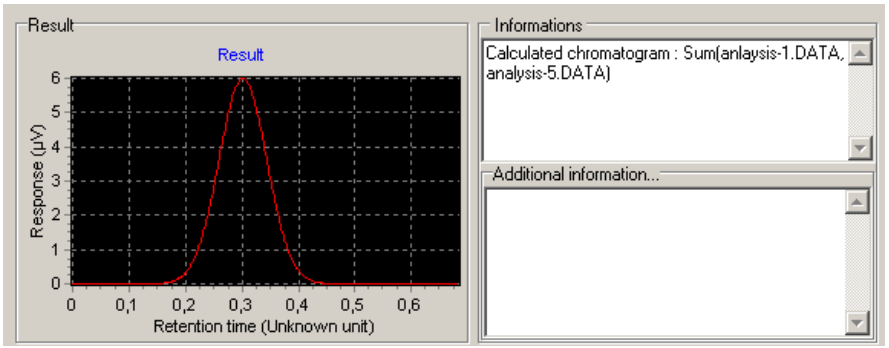
Addition

Two chromatogram plots can be added by selecting two chromatograms as operands, or add a value to all points of the chromatogram plot, then activate the Addition operator.

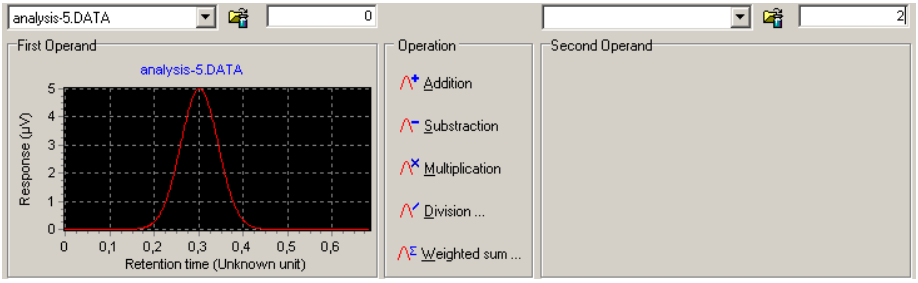
Chromatogram and Operator Selection: Two chromatograms



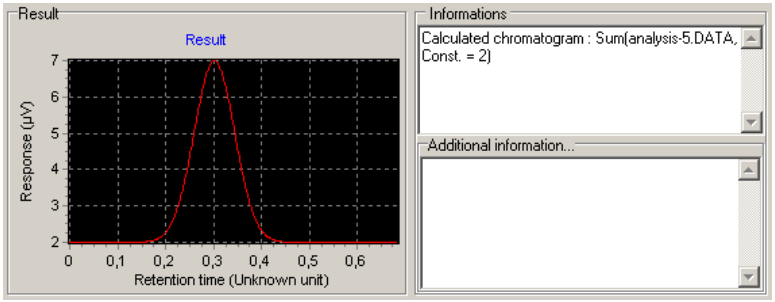
Result:



Chromatogram and Operator Selection: One Chromatogram and One Operator



Result:



Subtraction

Subtract one chromatogram from another chromatogram by selecting two chromatograms as operands, or subtract a value from all points of the chromatogram plot. Then the subtraction is performed by activating the operator.

NOTE: In case of subtraction of two chromatograms, the second one (second operand) is subtracted from the first one (first operand).

Multiplication

Multiply one chromatogram by another chromatogram by selecting two chromatograms as operands, or multiply all points of the chromatogram. The multiplication is performed by activating the

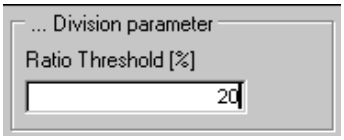
operator. If two chromatograms are multiplied, the signal value is multiplied point by point.

Division

Divide one chromatogram by another chromatogram by selecting two chromatograms as operands, or divide all points of the chromatogram. The division is performed by activating the

operator.

The ratio threshold % must be defined. The ratio chromatogram threshold determines a maximum value for ratio calculation when performing the “Division” function.



When performing the A/B division, if the signal intensity of the first chromatogram (A) multiplied by the ratio chromatogram threshold (in %) and divided by 100, is superior to the signal intensity of the second chromatogram (B), then the ratio is set to 0.

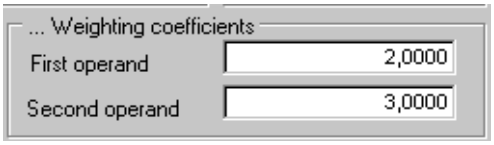
For example, if the ratio threshold is set to 20%, the ratio will be set to 0 if B<0.2A

This means that the intensity of the second chromatogram represents too small a percentage of the first chromatogram. So, the ratio chromatogram threshold sets the percentage of rejection.

Weighting Sum

This operation allows users to perform weighting addition operands. For example (2*First operand) + (3*Second operand).

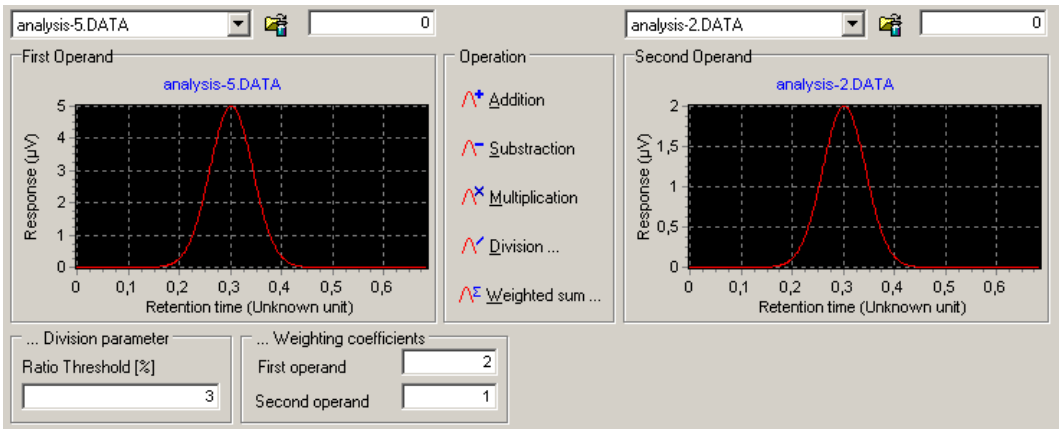
A user enters the first and second weighting coefficients, respectively for the first and second operand. These will be used to perform the sum.



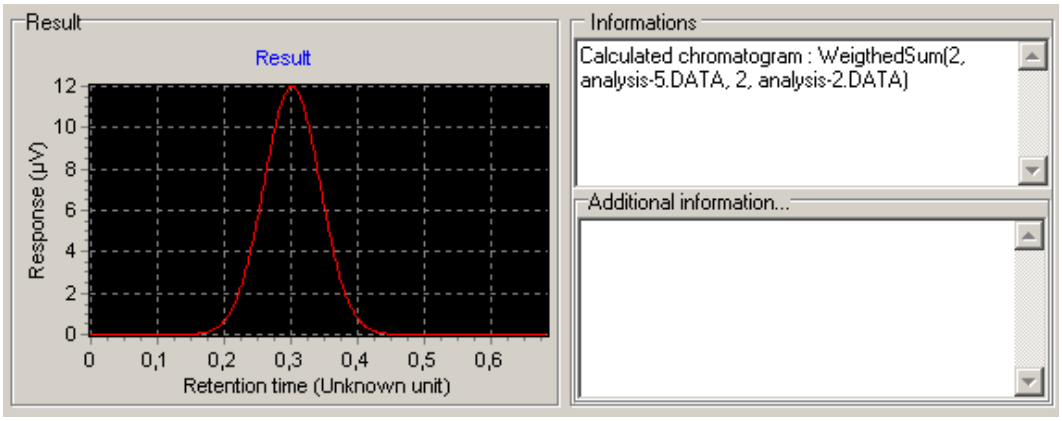
The

operator is then activated

Chromatogram and Operator Selection: Two Chromatograms with Weighting Coefficients.



Result:



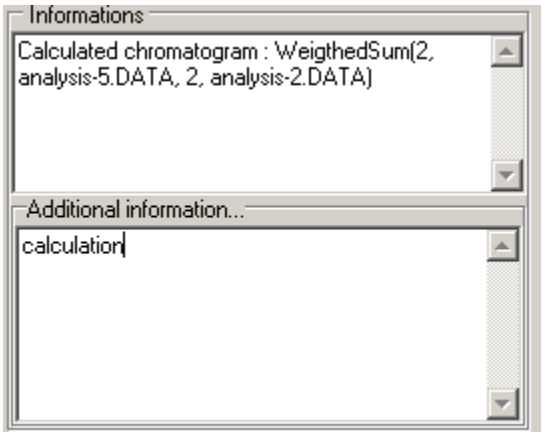
Generation of a Chromatogram Usable in CompassCDS

Saving the Generated Chromatogram

The virtual chromatogram generated can be saved as a .VIRT file. Then, it can be processed as a normal chromatogram in CompassCDS.

When the result is displayed at the bottom left part of the screen, select the button or the FILE / SAVE RESULT menu and enter a file name.

The text displayed in the Information field will be automatically saved with the chromatogram. The text corresponds to the description of the calculation which was processed to obtain the chromatogram. If a user wants to add more information, this is entered in the Additional information field.



The defined information will be displayed in CompassCDS at the chromatogram opening, in the Open / Save file box, and in the chromatogram properties.

Loading a Virtual Chromatogram in CompassCDS

After the calculation, the chromatogram displayed in the Result section can then be exported into CompassCDS.

Users can choose to either export the generated chromatogram while the Plug-in remains open:

Select the FILE/ OPEN RESULT IN COMPASSCDS menu or click on the button.

Or to export the generated chromatogram and automatically close the Plug-in:

Select the FILE/ GOING BACK TO COMPASSCDS WITH RESULTS menu or click on the button.

In both cases, the export chromatogram default name is ArithmeticChromatogram.VIRT.

NOTE: Once an exported chromatogram is open in CompassCDS, no other chromatogram can be exported from the Plug-in unless the first chromatogram is closed.

Returning to CompassCDS without Generating a Virtual Chromatogram

Select the button, or the FILE / CLOSE menu to come back to CompassCDS without any results.

The Plug-in is automatically closed.

CompassCDS
ASCII Import Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501486
Revision C

Contents

Introduction 3
Application Details 3
Converting One ASCII File 3
Converting Several ASCII Files 6
Opening Converted Files in CompassCDS 6

Introduction

This guide presents the CompassCDS ASCII Import Plug-in and describes configuration and use.

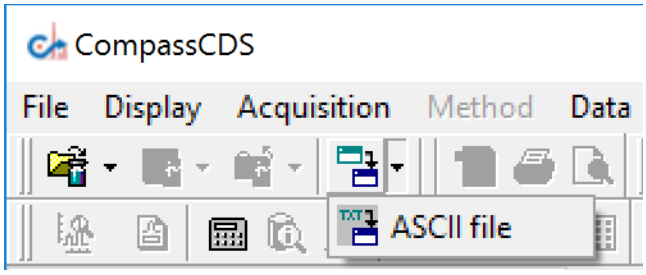
A plug-in is a small program that can process any kind of data on specific chromatographic files: global, group or peak information data. The plug-in data treatments have no influence on CompassCDS raw data.

The CompassCDS ASCII Import plug-in program converts ASCII data into CompassCDS data. It is installed during CompassCDS setup.

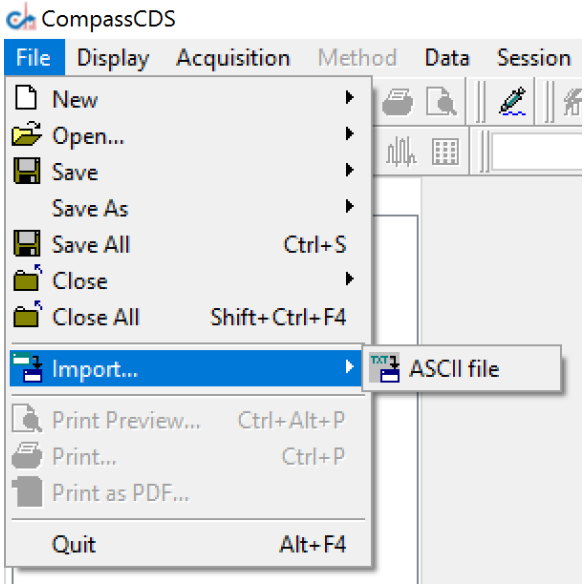
Application Details

Converting One ASCII File

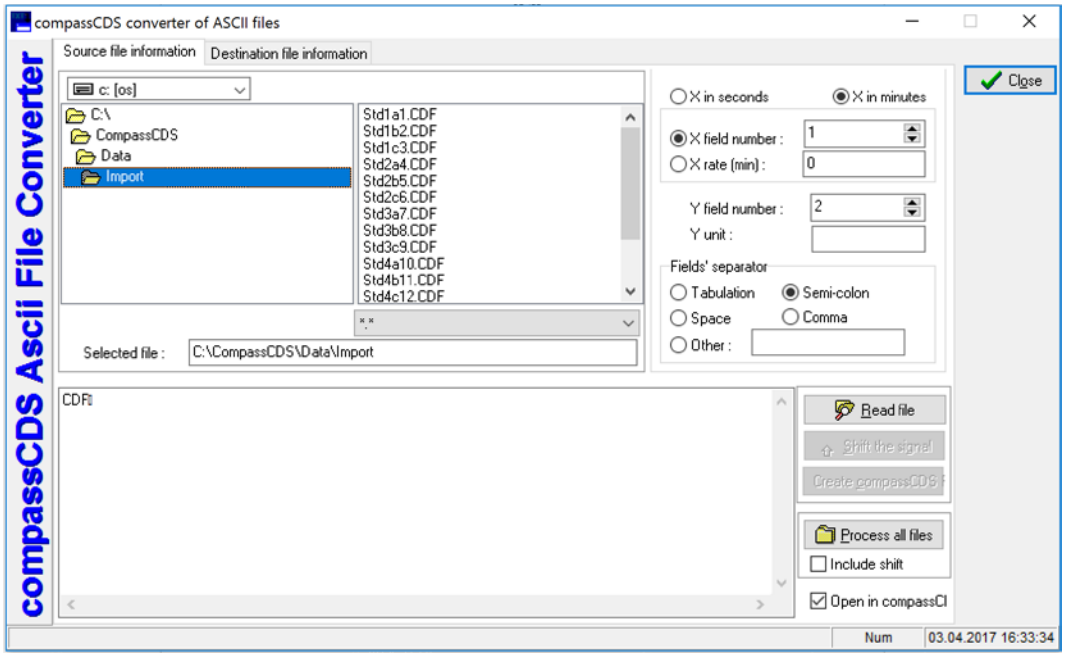
Select the ASCII file import option in the plug-in menu, in CompassCDS toolbar:



Or select File, Import option from the menu:



A new screen appears:



First, select the directory where the ASCII files are stored and then select the ASCII file to convert. The plug-in can convert .txt or .csv files into CompassCDS Data files.

Select the unit to be used for the X axis (minutes or seconds).

The user can select either the place where the X data are (by selecting the X field number option and then entering the column number) or the data rate (if no X data are available for example), and then can select the column number where X (or Y) data are listed. Enter the Y unit in the dedicated field.

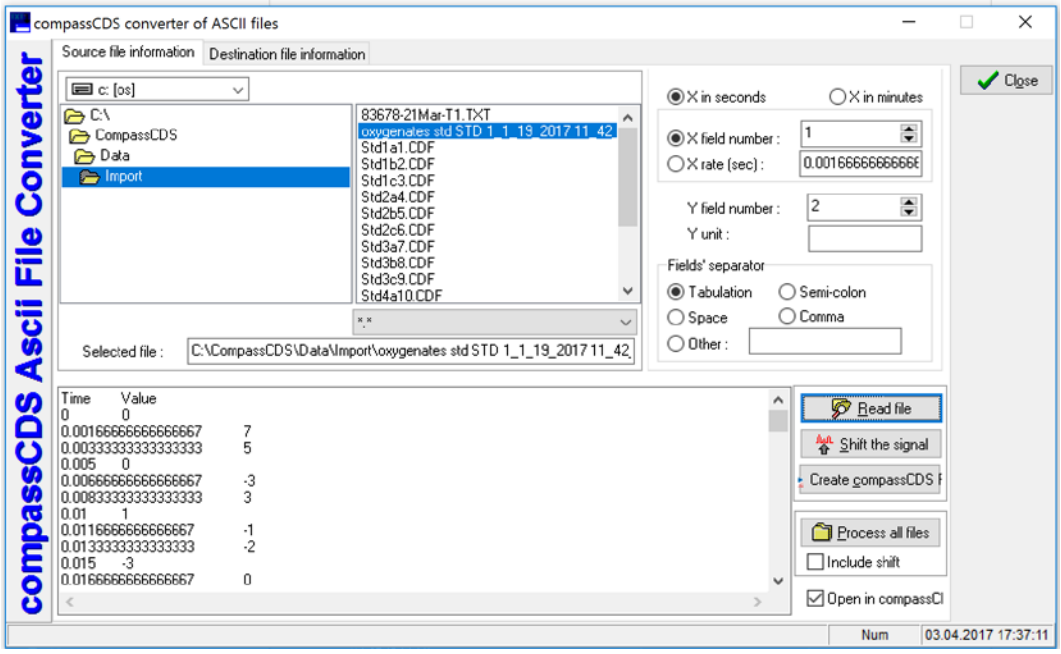
In the Field separator, select the item which separates the X and the Y data.

When the correct field separator is selected, click on the

button. Two buttons appear, (

and

) and the correct X rate is displayed in the dedicated field.



The raw data are displayed in the lower part of the screen.

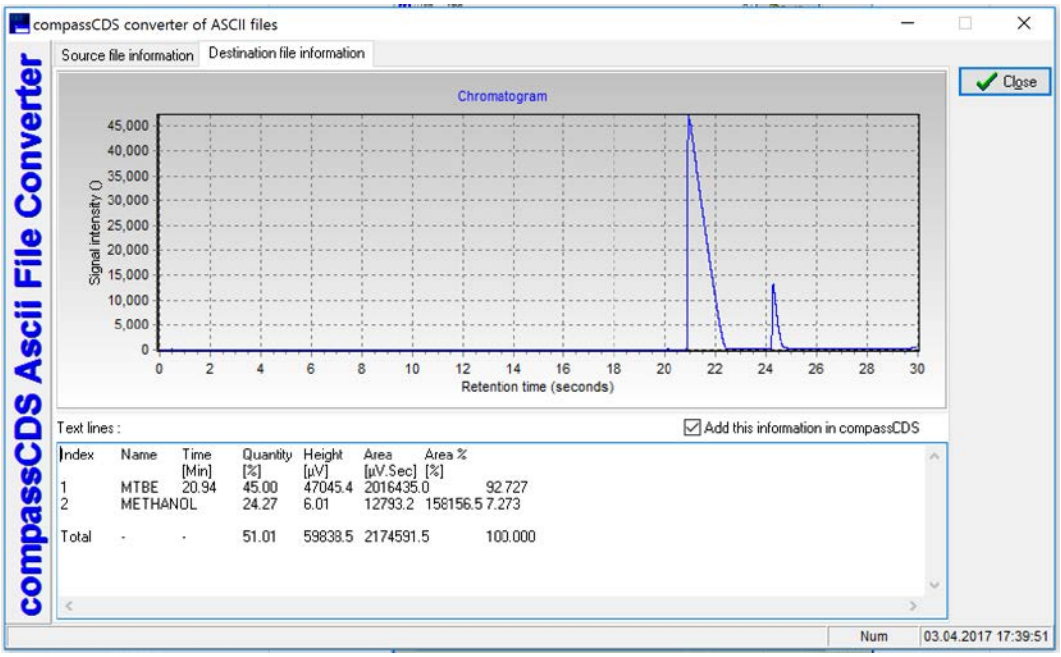
When the

button is clicked, the signal is automatically shifted so that the coordinates of the first point is (0,0). This shift will be included in the Data file if the corresponding Include shift box is checked.

When the user clicks on the

button, the current file will be processed. The corresponding CompassCDS.DATA file is created and opened in CompassCDS if this option is checked.

Click on the Destination file information tab. The chromatogram is displayed according to the different parameters fixed in the Source file information tab.

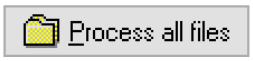


Users can enter information in the Text lines area. This information will be added in the Data file if the Option 'Add this information in CompassCDS' box is checked.

Converting Several ASCII Files

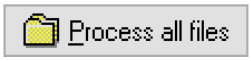
First select the directory where the ASCII files are stored and then select the ASCII files to convert.

Then select the unit of X axis (minutes or seconds). In the X field number (or Y field number), choose the column number where X (or Y) data are listed. Enter the Y unit in the dedicated field. In the Field's separator, choose the item that separates the X and the Y data. All these parameters must be the same for all the ASCII files selected.

To create Data files, click on the 

button. All the selected files are converted into Data files. If the Option "Open in CompassCDS" is checked, all converted files will be opened in CompassCDS after the processing.

Opening Converted Files in CompassCDS

When a user clicks on the 

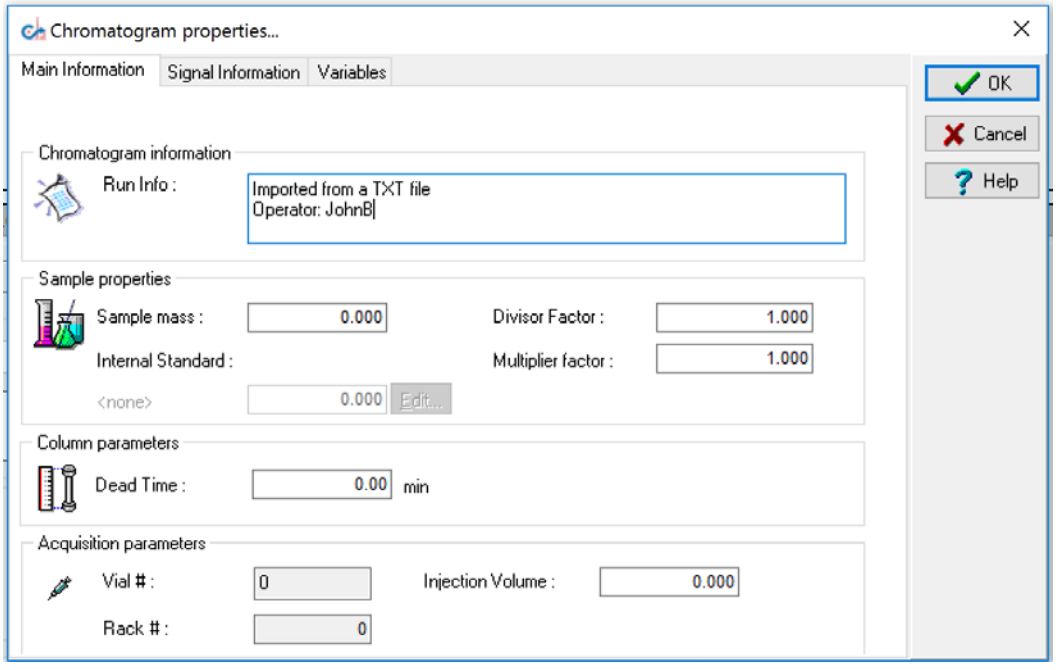
or the

buttons, data files are generated. If the option "Open in CompassCDS" is checked, the data file(s) are immediately opened in CompassCDS (after CompassCDS processing). After conversion, the generated files are identical to standard CompassCDS data files.

If a user has entered information in the Text lines area and if the Option "Add this information in CompassCDS" box is checked, this information appears in:

- The Description field in the open box
- The runinfo variable
- The Description area of the chromatogram properties.

The following screen gives an example of description entered by user in the ASCII import plug in:



CompassCDS
Instant View Plug-in
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501589
Revision B

Overview

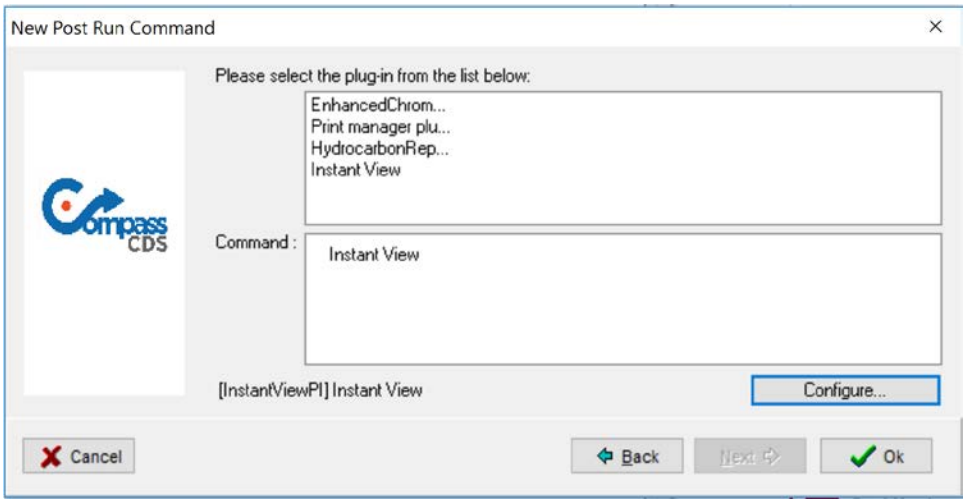
This plug-in provides users with the ability to have Chromatogram files automatically load into the CompassCDS Data view after either a Quick Start or a Sequence run has been completed. This eliminates the need for users having to search for files that have just been run and which they wish to review.

Installation and Setup

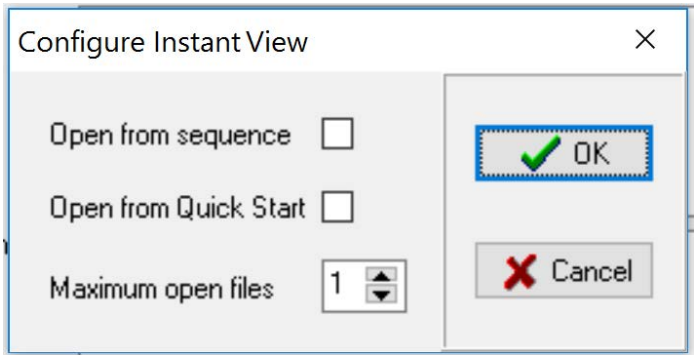
To install the Instant View plug-in, run the Setup.exe program. The plug-in DLL (“InstantViewPI.dll”) will be installed in the CompassCDS Client directory.

To use the Instant View plug-in, it must be added to the post-run section of a CompassCDS method. In a multi-channel method, it must be added only to the last channel. It should also always be the last item in a post-run section.

In the post-run section of a method, click the “Add” button and select “Compass Plug-in” as the program type. The following window will appear:

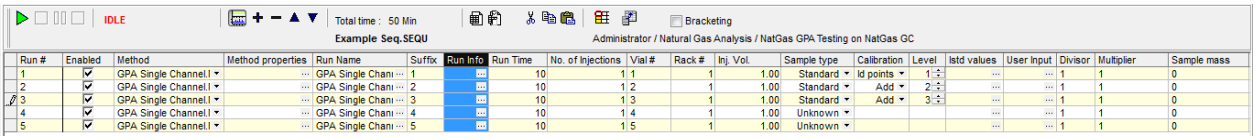


Select Instant View from the list of available plug-ins. Then click the “Configure” button. The following selection will appear:

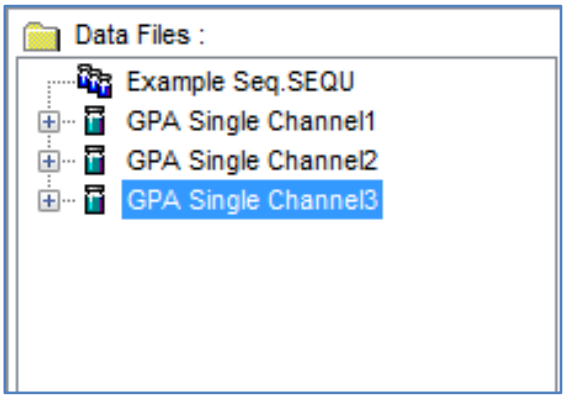


Normally both the Open from sequence and the Open from Quick Start options should be checked by the user. CompassCDS data files will only be automatically loaded into the Data view following an acquisition, either via Quick Start or a sequence as (shown below) and will not be loaded after a reprocessing. Once the appropriate choices have been made, close both dialogues by clicking the “OK” buttons.

In the sample sequence shown below, each line of the sequence will generate a data file which will be automatically loaded into the Data view for review/reprocessing by the user.



Run #	Enabled	Method	Method properties	Run Name	Suffix	Run Info	Run Time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type	Calibration	Level	Istd values	User Input	Divisor	Multiplier	Sample mass
1	☑	GPA Single Channel.I	...	GPA Single Chani	1	...	10	1	1	1	1.00	Standard	Id points	1	...	...	1	1	0
2	☑	GPA Single Channel.I	...	GPA Single Chani	2	...	10	1	2	1	1.00	Standard	Add	2	...	...	1	1	0
3	☑	GPA Single Channel.I	...	GPA Single Chani	3	...	10	1	3	1	1.00	Standard	Add	3	...	...	1	1	0
4	☑	GPA Single Channel.I	...	GPA Single Chani	4	...	10	1	4	1	1.00	Unknown			...	...	1	1	0
5	☑	GPA Single Channel.I	...	GPA Single Chani	5	...	10	1	5	1	1.00	Unknown			...	...	1	1	0



CompassCDS
1-Button Interface Installation and User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501592
Revision C

Contents

Understanding the 1-Button Interface 3
Installing and Configuring the 1-Button Interface 3
  Installing CompassCDS 3
  Installing the 1-Button Interface 3
Logging into the 1-Button Interface as an Administrator 5
Configuring Analysis Types using the Administration Setup 5
Logging into and Running the 1-Button Interface as an Operator 10
Executing Unknown Sample runs 12
Executing Calibration and Verification runs 13
Executing Continuously Looping Analyses 14

Understanding the 1-Button Interface

The 1-Button plug-in interface enables users to operate gas chromatographs being controlled by the Scion Instruments CompassCDS software and generate results without having to access the CompassCDS software application itself. 1-Button uses the same log-on, audit trail and security features associated with CompassCDS and has been designed to provide plant operator level users with a straightforward and intuitive interface that enables them to quickly set up and run routine product sample analyses and then generate the associated results report with one button click.

The 1-Button interface can be installed and configured by any CompassCDS administrator level user who can then set up fully automated, multi-injection calibrations, followed by verification runs (if required) and unknown sample analyses either as single injections with/without autosampler vial position support or as continuously looping analyses. Once configured, all of these can be run by simply selecting and clicking on the appropriate icon in the GUI.

Installing and Configuring the 1-Button Interface

Installing CompassCDS

The CompassCDS software should be installed and configured in accordance with the procedures described in the CompassCDS software installation guide found in the root folder on the CompassCDS DVD. Once installed, a 1-Button Administrator and a 1-Button Operator user type with accompanying user profiles (Figure 1) should be configured in the Configuration Manager application. It is also recommended that all user profiles be assigned at least a $Year4\$Month2 folder token.

Installing the 1-Button Interface

The 1-Button application can be installed by locating and running the Setup.exe found in the Add-ons\1-Button folder on the CompassCDS DVD. Once the installation has completed, the migration tool must be run to integrate the 1-Button application with CompassCDS. To run this tool, the user should click on the InsertCustomProgramRights.bat file found in the Add-ons\1-Button\migrate folder and then press Enter. Once this tool has been run, it will be possible to assign Administrator and Operator user profile rights from within the Configuration Manager as shown in Figure 2.

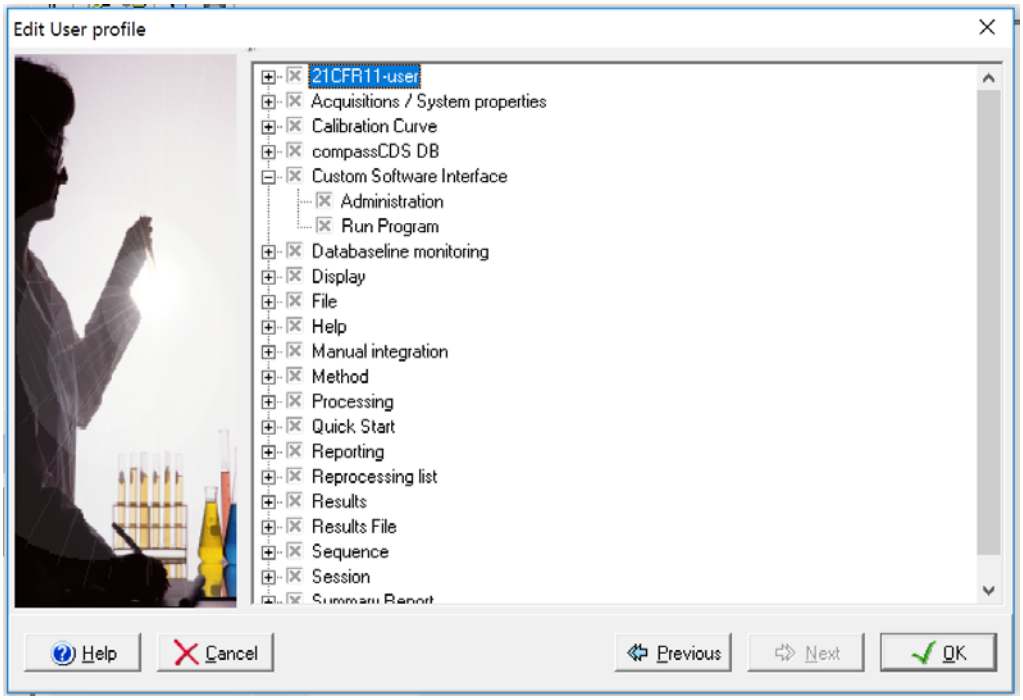


Figure 1 1-Button Administrator level User Profile

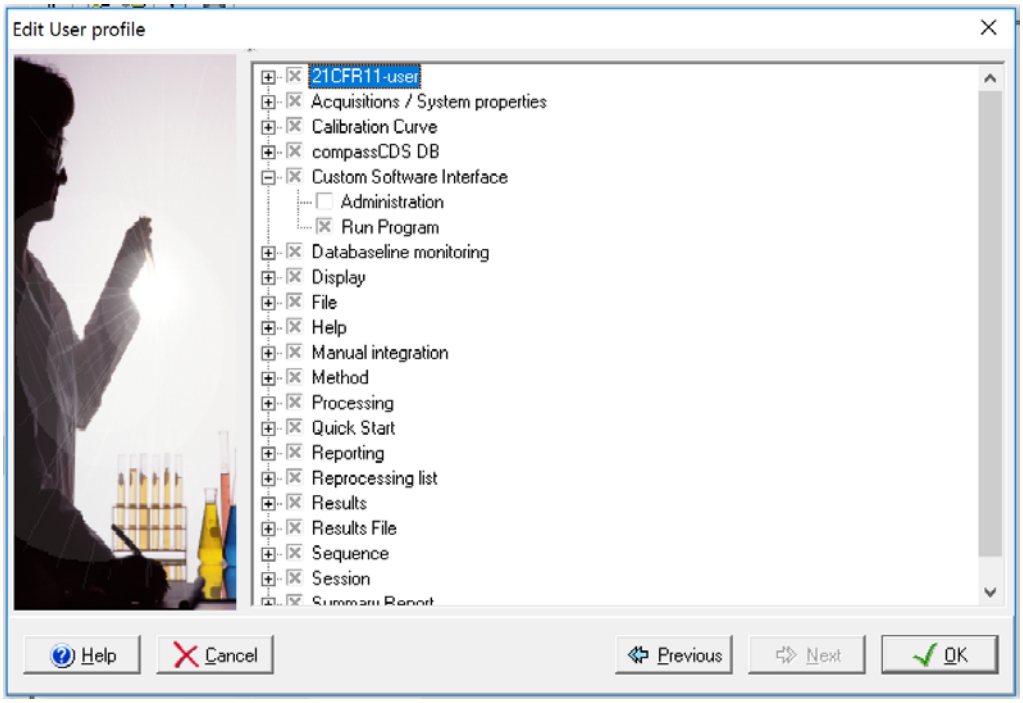


Figure 2 1-Button Operator level User Profile

Logging into the 1-Button Interface as an Administrator

1-Button Administrators can access the 1-Button application by double clicking on the 1-Button desktop icon . This will bring up a login dialogue similar to that shown in Figure 3 below. Administrators can then enter the default CompassCDS Administrator login, select a Group, Project and if required the associated Administrator password. This dialogue will retain the information from the last logged on user.

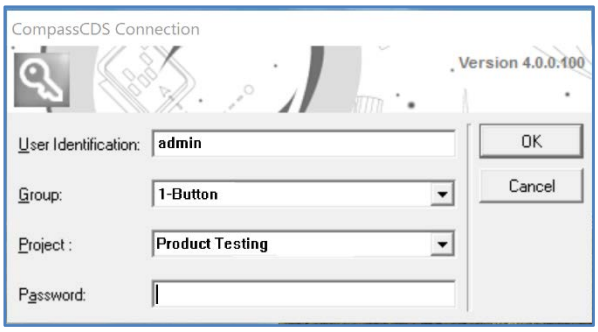
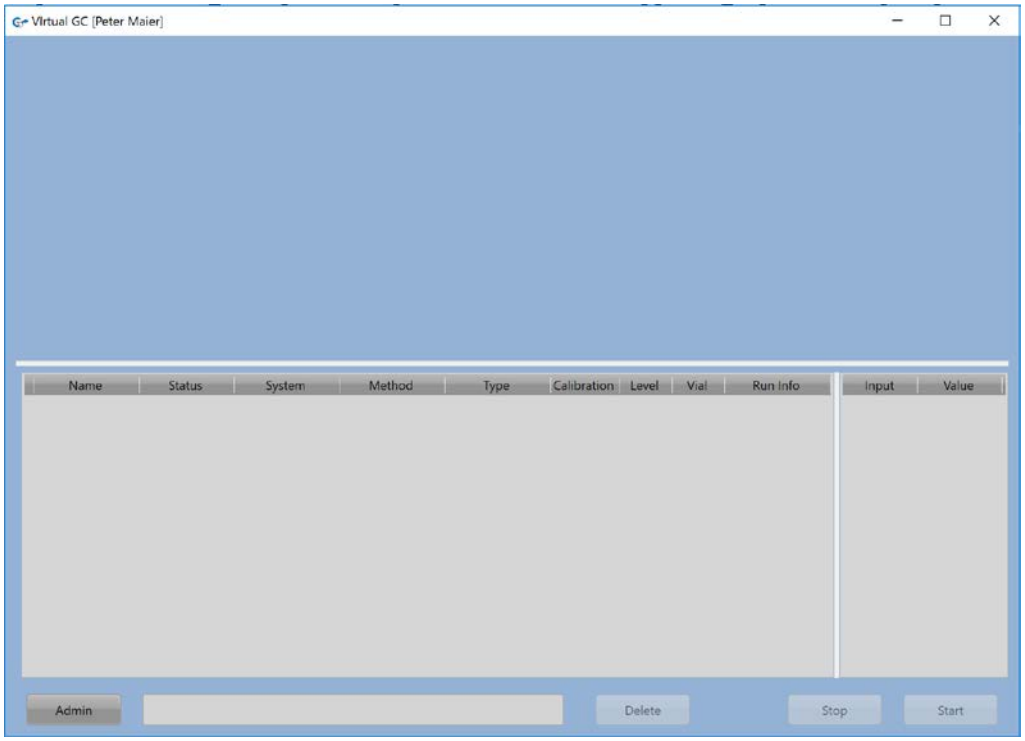


Figure 3 1-Button Administrator Login dialogue

Configuring Analysis Types using the Administration Setup

When logging into the 1-Button application for the first time, a blank GUI similar to the one shown in Figure 4 below will appear.



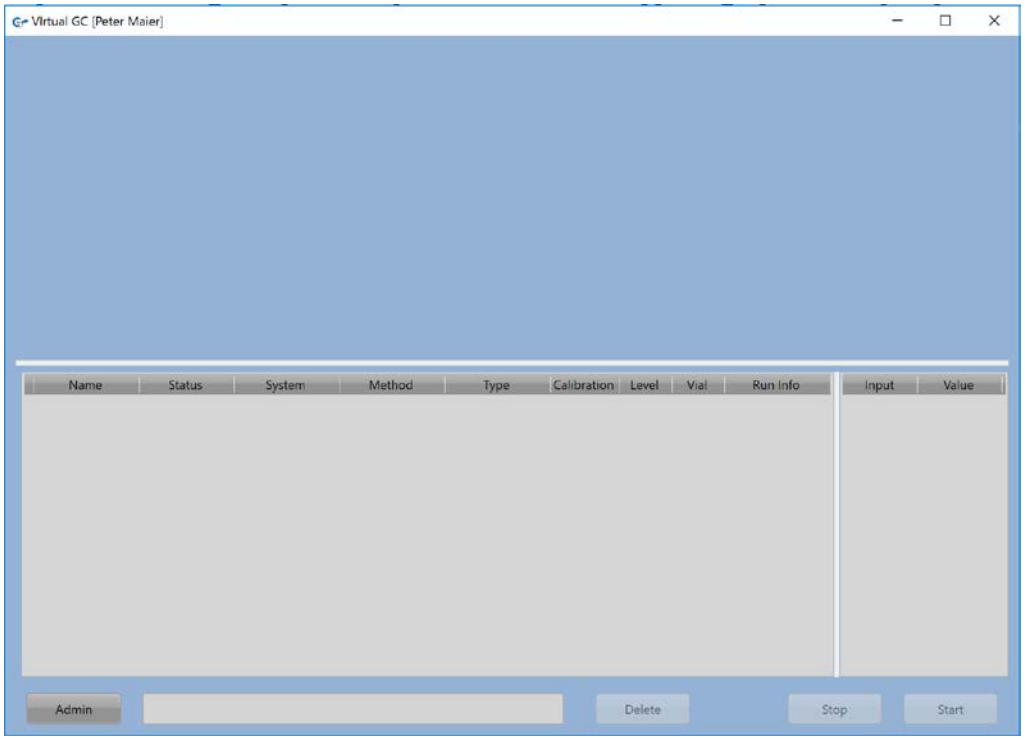
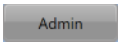


Figure 4 1-Button main GUI

Click the  button to bring up the 1-Button Administration Setup GUI shown in Figure 5.

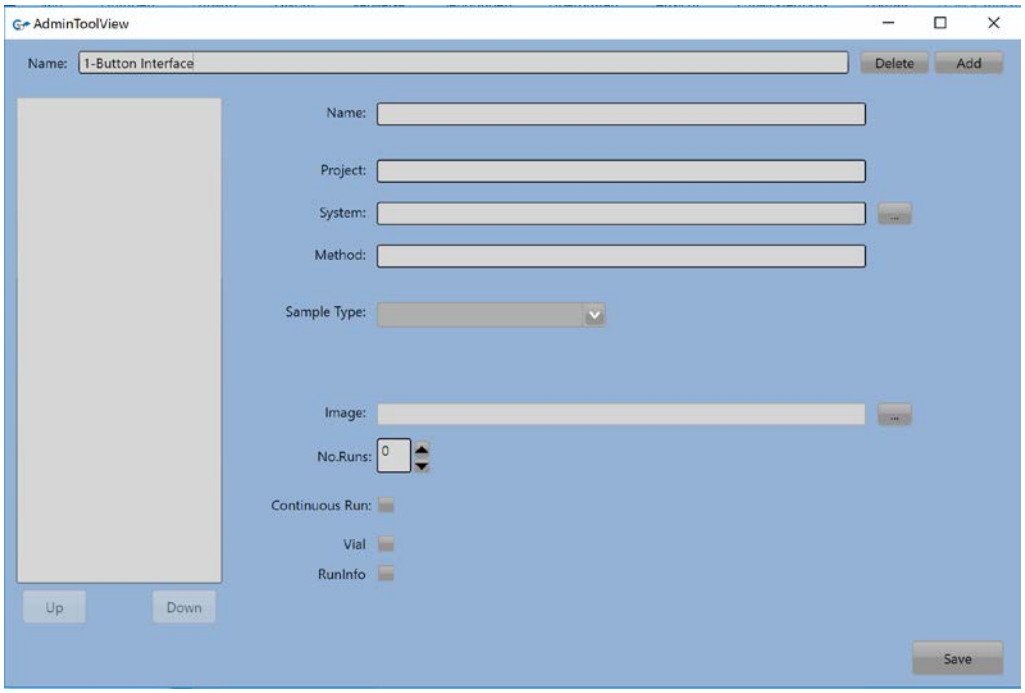


Figure 5 1-Button Setup GUI

A CompassCDS Method (.METH) is the item that needs to be selected in order to create a new analysis type and to be able to populate the Setup fields. It is assumed that the CompassCDS method being selected is complete, i.e., this method contains a Peak ID table, a valid calibration curve, user input variables (if required) and a configured report style. If not, it is still possible to complete the configuration of an analysis type in the 1-Button setup dialogue and finish editing the

CompassCDS method directly in CompassCDS at a later stage. An analysis type is set up from within the Setup Dialogue pane as follows:

1. Click the Add button and enter a name for the analysis, for example, Product QC in the Name: field.
2. Click on the ... icon and select the Method to be used for the analysis.
3. Select the Sample Type (Unknown, Standard, Blank, Control).
4. Select a suitable icon by clicking on the image ... icon and navigating to the icons folder.
5. Select the number of runs per analysis
6. If the analysis involves continuous looping, check this option and enter the wait time (in minutes) between samples
7. Click the Save icon and the analysis name will appear in the left-hand column as shown in the examples displayed in Figure 6.

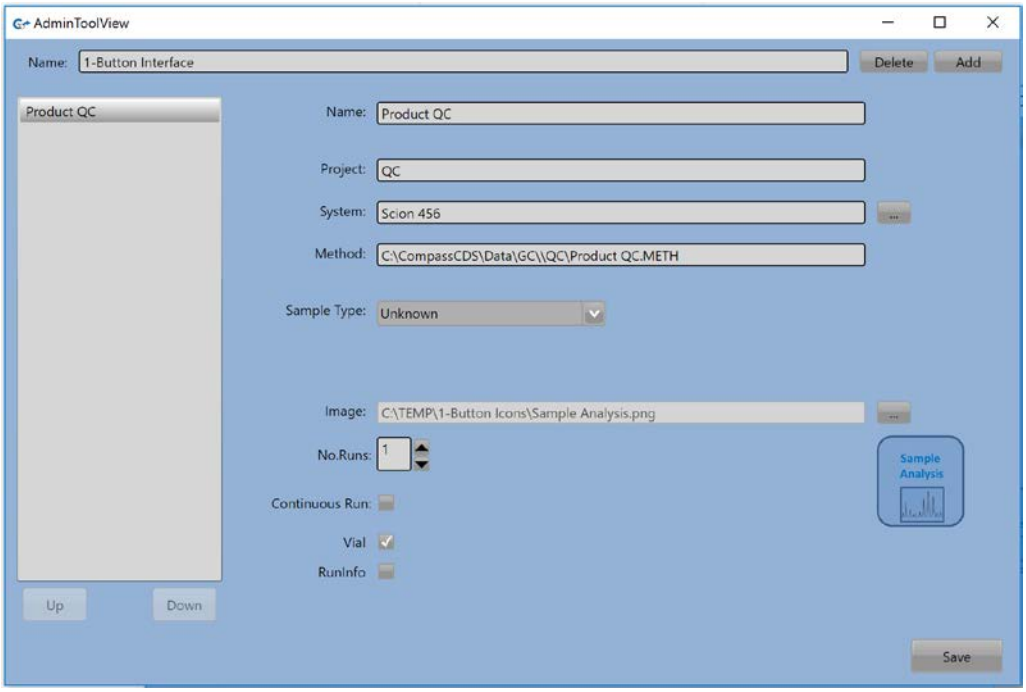


Figure 6 Example Setup for an Unknown Sample analysis

A Multi-level, multi-replicate calibration setup would look similar to the layout shown in Figure 7.

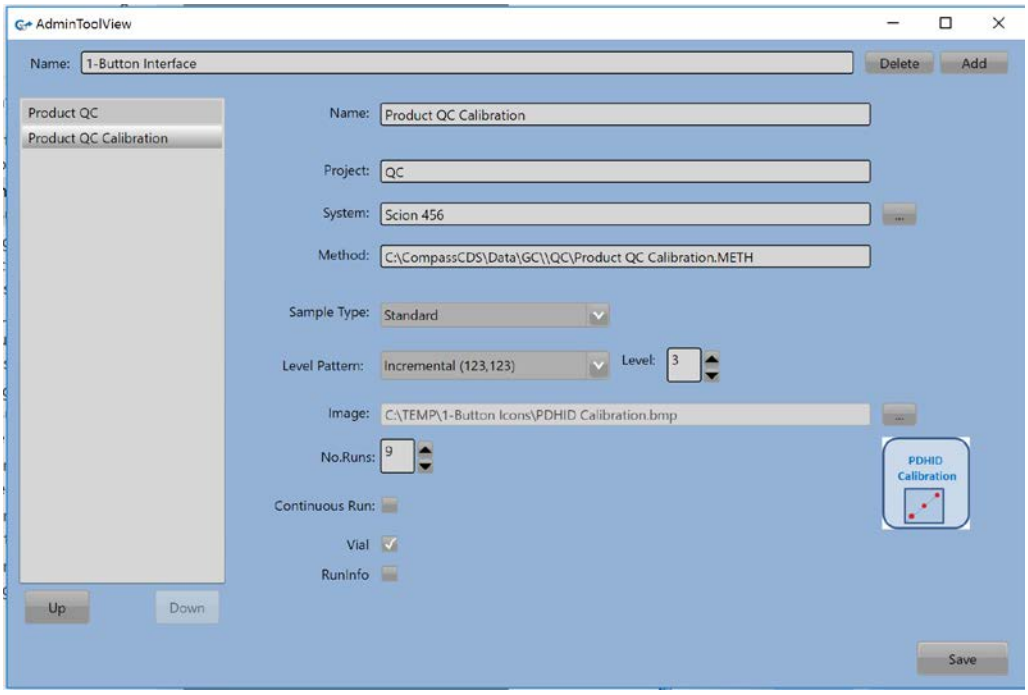


Figure 7 Example Setup for Calibration Standards (3 levels, three replicates per level)

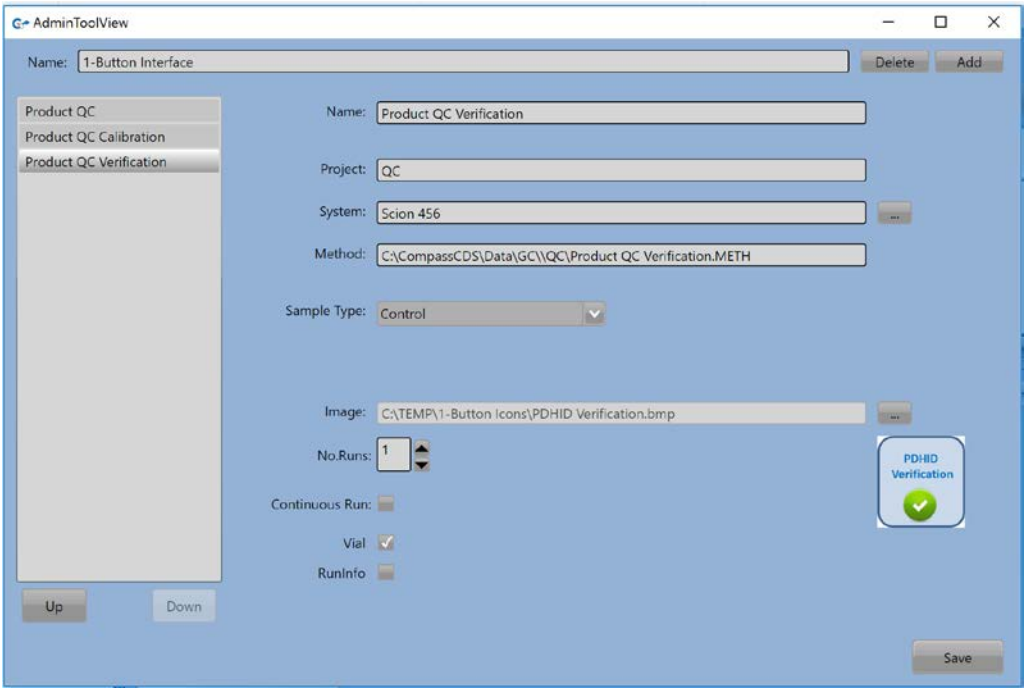


Figure 8 Example Setup for Calibration Verification analysis

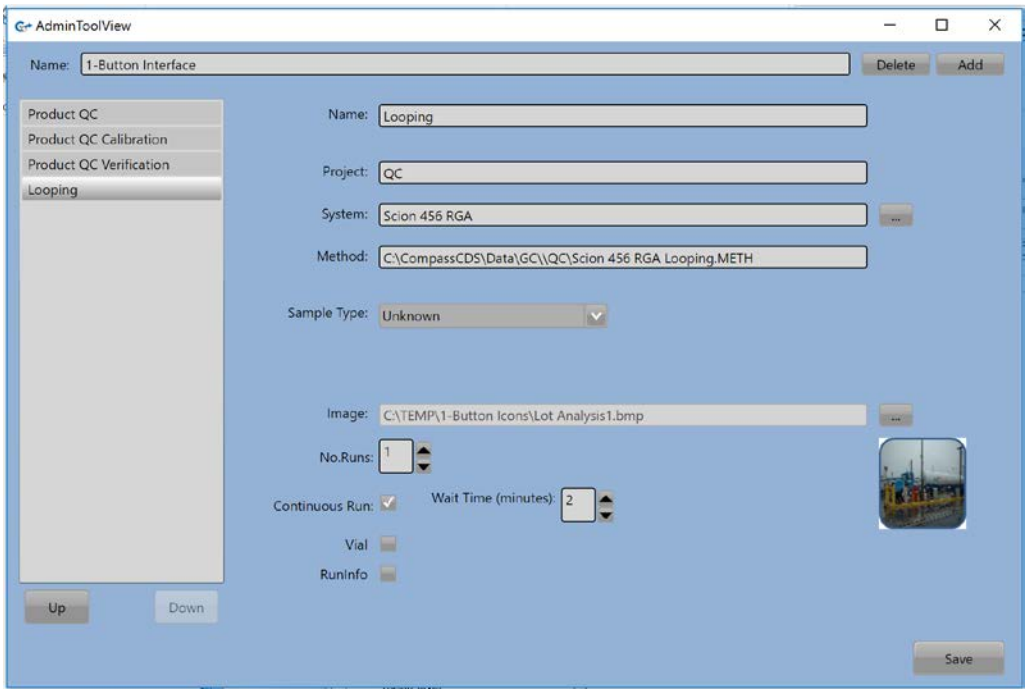


Figure 9 Example Setup Dialogue for a Continuously Looping analysis

Each one of these Setup Dialogue panes is represented by an icon in the 1-Button GUI and it is possible to change the order of these icons using the Up and Down buttons as shown in Figure 10.

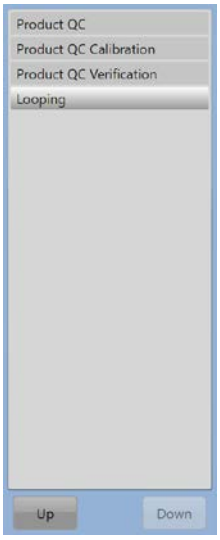


Figure 10 Analysis type icon order list

Clicking on the button will close the Administration setup dialogue and return to the 1-Button main GUI as shown in Figure 11.

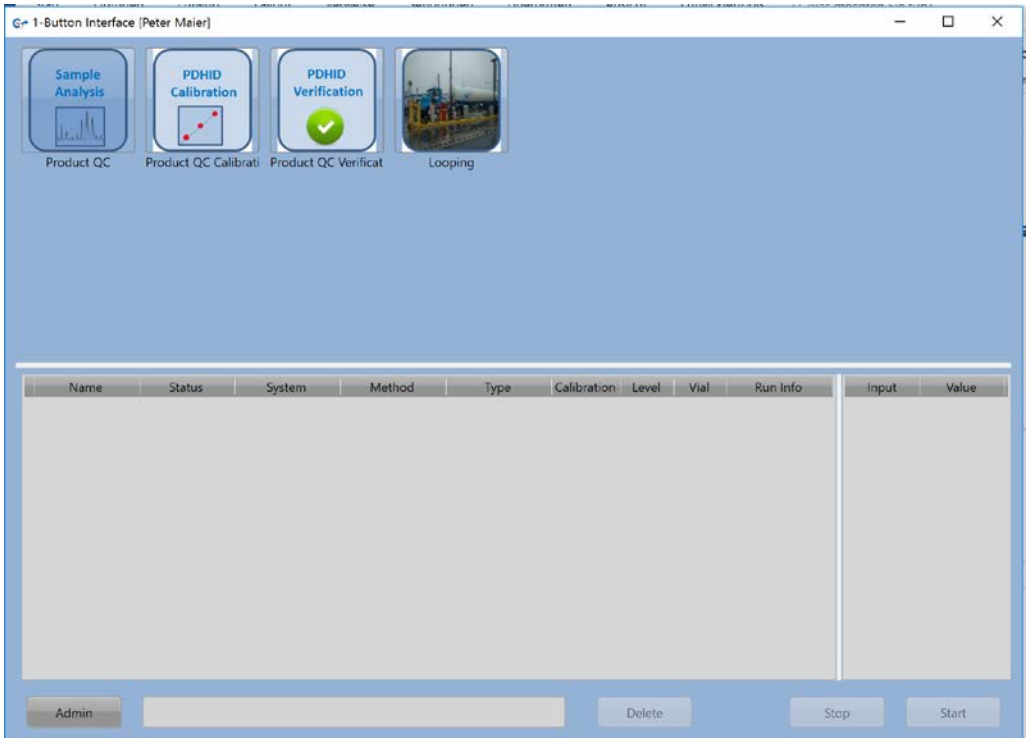


Figure 11 Configured 1-Button main GUI with icons for Product QC, Calibration, Verification and Looping Analyses

Logging into and Running the 1-Button Interface as an Operator

Operators can access the 1-Button application by double clicking on the 1-Button desktop icon . This will bring up the login dialogue shown in Figure 12. Operators can then enter the default operator login User Identification, select a Group, Project and if required the associated operator password. This dialogue will retain the information from the last logged on user.

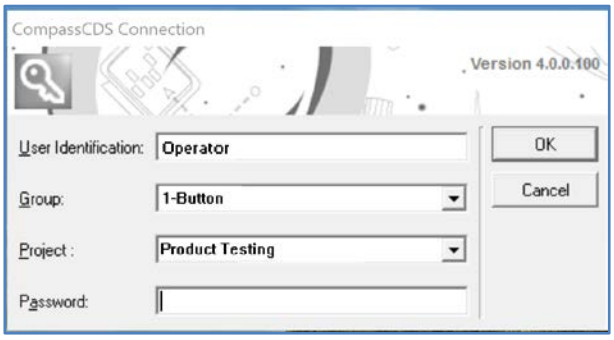


Figure 12 1-Button Operator Login dialogue

The 1-Button main GUI will appear as shown in Figure 13.

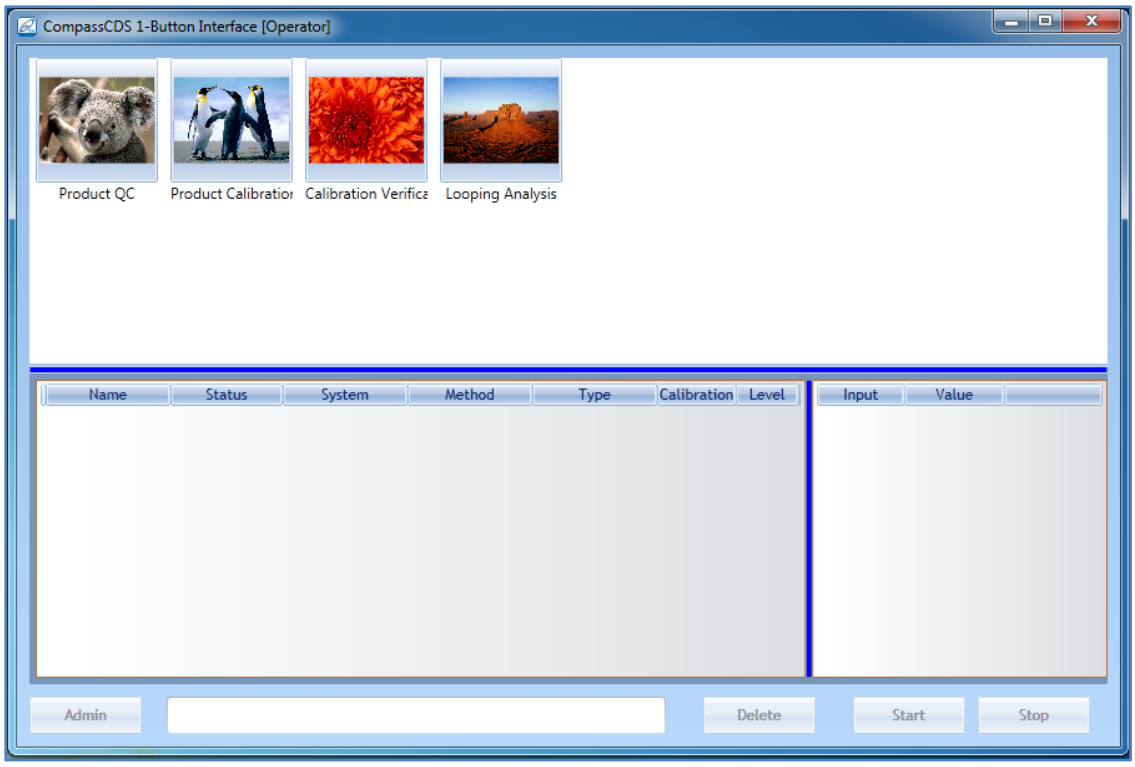


Figure 13 1-Button main GUI with icons for Product QC, Calibration, Verification and Looping analyses

Operators can click on any of the visible icons to load and run pre-configured Analysis types including:

- Product Analyses
- Calibration or re-calibration sequences
- Calibration verification runs
- Looping analyses for continuous sampling applications

In addition, operators can add user input variable information for specific Analysis Types in the right hand pane and have the ability to stop/start/delete runs.

Executing Unknown Sample runs

Routine product sample QC analyses can be setup and run using the 1-Button interface. The 1-Button GUI makes this a simple operation that requires clicking on the following icon either once for a single analysis or multiple times if more than one sample is to be run as shown in the example below.

To initiate a Product QC run, the operator should click once on the Product QC

icon and a single line the GUI as shown in figure 6.1 below. Two mandatory user input variables, (Batch No: and LIMS No:) have been added to this method and the operator will be required to enter the relevant information in order to proceed. Once a Batch and LIMS number have been entered, the operator can click the

button at this point and the analyses will proceed. Running analyses can be viewed by logging into CompassCDS and navigating to the Systems view.

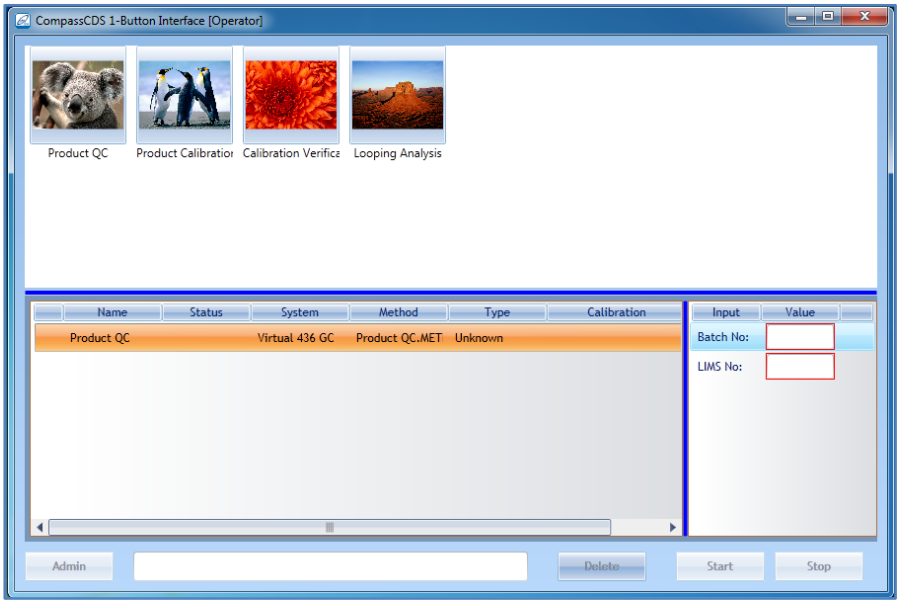


Figure 14 Example Product QC analysis with mandatory user entry variables

Once the run completes, the corresponding line in the 1-Button GUI will disappear and the resultant chromatogram can be reviewed (if required) in the CompassCDS Data view.

Executing Calibration and Verification runs

To generate calibration (or re-calibration) curves and to then automatically calculate the percent recovery values for each component being analyzed, an operator simply needs to click once on the Product Calibration and once on the Calibration Verification icon. A calibration sequence of 9 runs followed by a verification run will automatically be added to the GUI as shown in Figure 15. The operator can click the button and at this point and the displayed analyses will proceed.

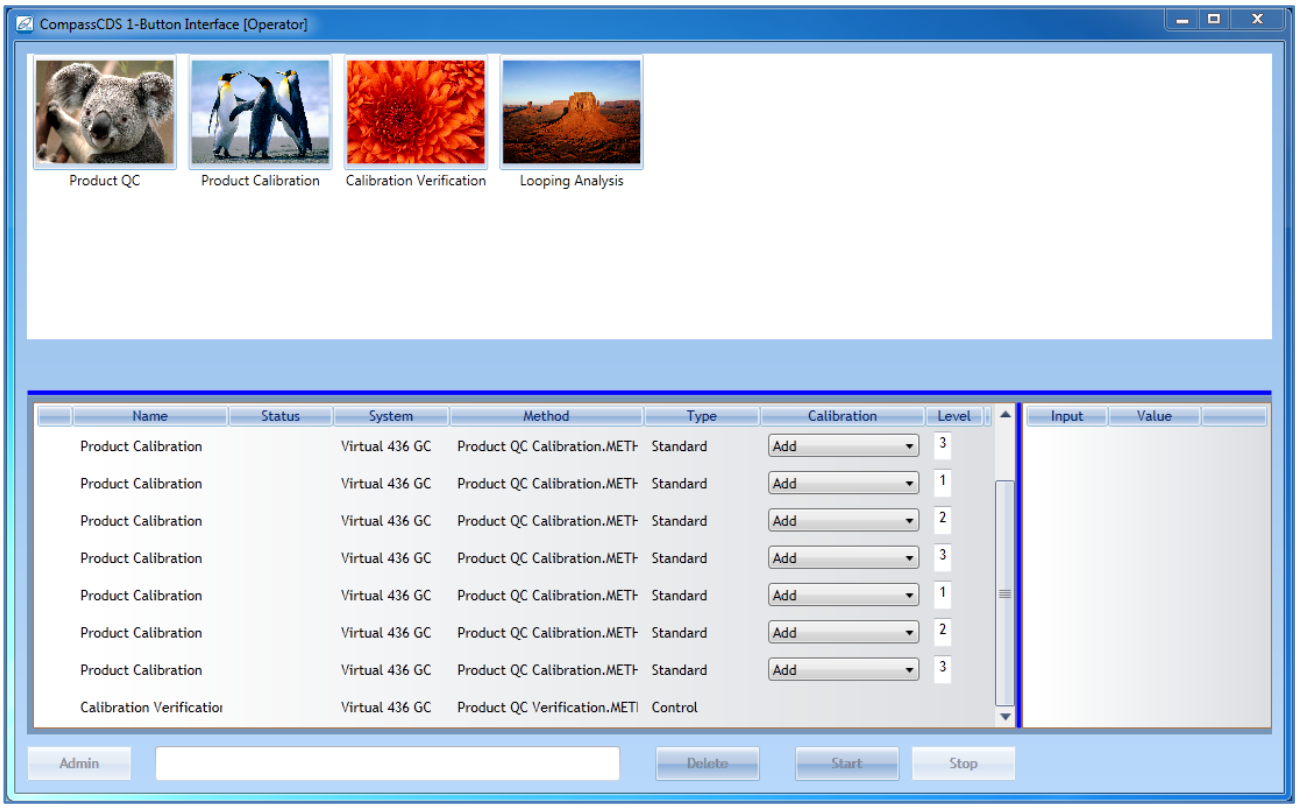

CompassCDS 1-Button Interface [Operator]
Product QC
Product Calibration
Calibration Verification
Looping Analysis
Name
Status
System
Method
Type
Calibration
Level
Input
Value
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 3
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 1
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 2
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 3
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 1
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 2
Product Calibration Virtual 436 GC Product QC Calibration.METH Standard Add 3
Calibration Verificatio Virtual 436 GC Product QC Verification.METI Control
Admin
Delete
Start
Stop

Figure 15 Three level, 3 replicate calibration sequence (9 runs) with a verification run

Executing Continuously Looping Analyses

To set up a continuously looping analysis, an operator simply needs to click once on the Looping Analysis icon. A line will automatically be added to the GUI as shown in Figure 16. The operator can click the button and at this point and the displayed analysis will proceed until the operator clicks the Stop button OR another sample such as a Product QC is added, in which case the continuously looping analysis will pause at the end of the current run and the added sample will then run. Once the Product QC analysis has completed, the looping analysis will continue once more.

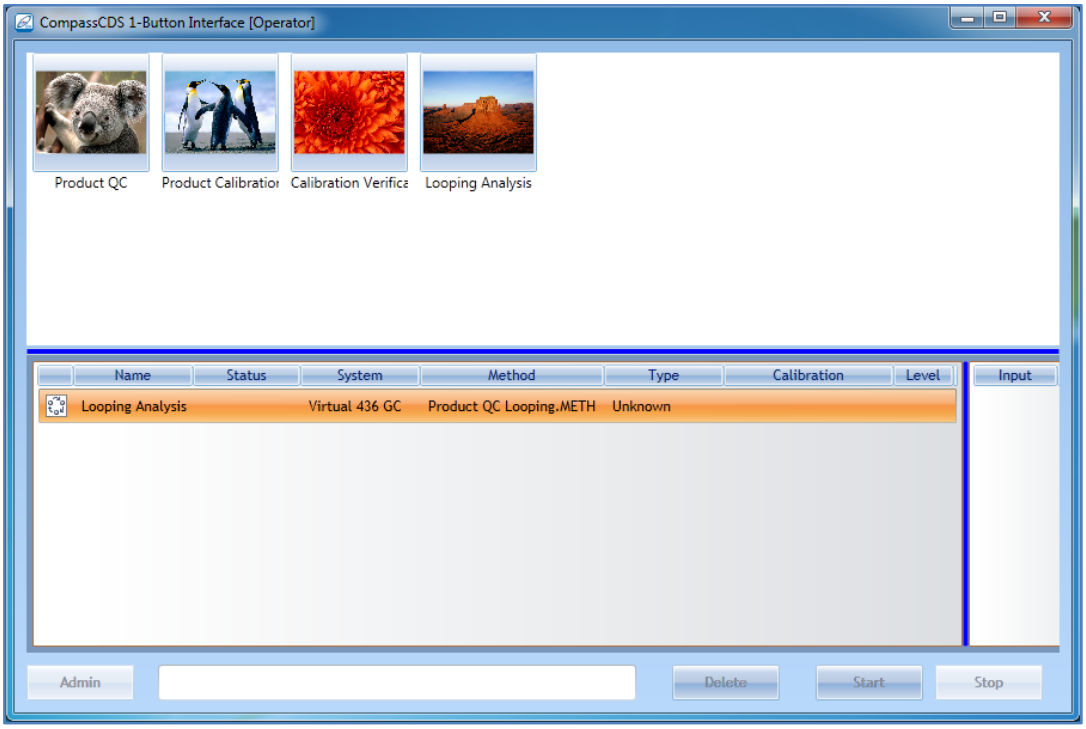


Figure 16 Continuously looping run

CompassCDS ChromSync User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501544
Revision A

Contents

Overview Presentation 3

Installation and configuration 4

- Configuration requirements 4
- Installation instructions 4
  - UNINSTALLATION: 4
  - INSTALLATION: 4

Getting started with CompassCDS ChromSync 5

- Diagram of the application 5
- Using CompassCDS ChromSync Plug-in 5
  - Creating and saving a reference 5
  - Comparison 6

Details of the application 9

- The different file types 9
- Choosing a Reference 10
  - How Can You Define a Reference? 10
  - Area Tolerance 10
  - The Success Criterion 13
- Sample Choice and Processing 14
  - Choosing the Chromatograms to Compare 14
  - From Windows desktop: the sequence list 14
  - Matching 20
- Displaying the Results 25
  - The Time Shift 25
  - Peak Areas 26
  - Results Peak by Peak 27
  - Global Estimate of the Comparison 28
  - Modifying the Result Display 29
- Comparison Report 34
  - Comparison Report Format 34
  - Customizing the Report 40
- Excel Export 40
  - Customizing the report 40
  - Export 41
- ChromSync summary 41
- Specific Case: Retention Indices 43

Tips and Examples 45

- Working with Large Directories 45
- Influence of Temporal Tolerance 45
- Influence of the Shift Sign 46
- Influence of the Initial Shift 47
- Sensitive Areas within Chromatograms 48
  - Example #1 48
  - Example #2 49

Overview Presentation

CompassCDS ChromSync software compares a reference chromatogram with a sample chromatogram to find the reference peaks in the sample chromatogram. CompassCDS ChromSync identifies matching peaks as well as missing peaks.

Whether two peaks match or not is decided according to two criteria defined by the user: the first one concerns the *retention time*, the second one concerns the areas.

Two peaks match if their retention times and areas are similar. However, in a few rare cases, the temporal tolerance criterion cannot be satisfied but the peaks are nevertheless matched. This kind of match is called “out of temporal tolerance.”

The processing of chromatograms (which must be correctly integrated) consists of two steps:

1. The first step of processing is to set the references associated with a reference chromatogram: for each peak, identified by its retention time, an area percentage tolerance is defined. The names, the retention times, areas and area tolerances should be saved in a reference file (CompassCDS ChromSync Reference module). This Area tolerance has no influence on the peaks matching, but makes it possible for the user to define the accepted error percentage on the matching peak areas.

2. The second step is the comparison of an unknown chromatogram with the reference chromatogram. This comparison uses the reference parameters saved in the reference file. Other comparison parameters can be defined and the application couples the peaks. The quality of the match is displayed in this second module (CompassCDS ChromSync Comparison module). The two parameters temporal tolerance and the maximum error on area percentages are considered. The area tolerance parameter saved in the reference file shows tolerance error percentage by colors.

CompassCDS ChromSync can be launched:

- From the Windows start button or desktop.
- From CompassCDS.

The *Getting Started* section will help you identify the CompassCDS ChromSync basic steps. The *Detail of the Application* section lists all the features of the software.

Installation and configuration

Configuration requirements

CompassCDS ChromSync only runs with Windows XP, Windows Vista, Windows7, and Windows 10 (32 and 64 bits).

CompassCDS ChromSync requires a minimum of 25Mb on your hard disk.

CompassCDS ChromSync requires administrator privileges for installation.

Installation instructions

Uninstallation

If a previous version of ChromSync (< 1.3 version) is already installed on your computer, uninstall before proceeding with installation.

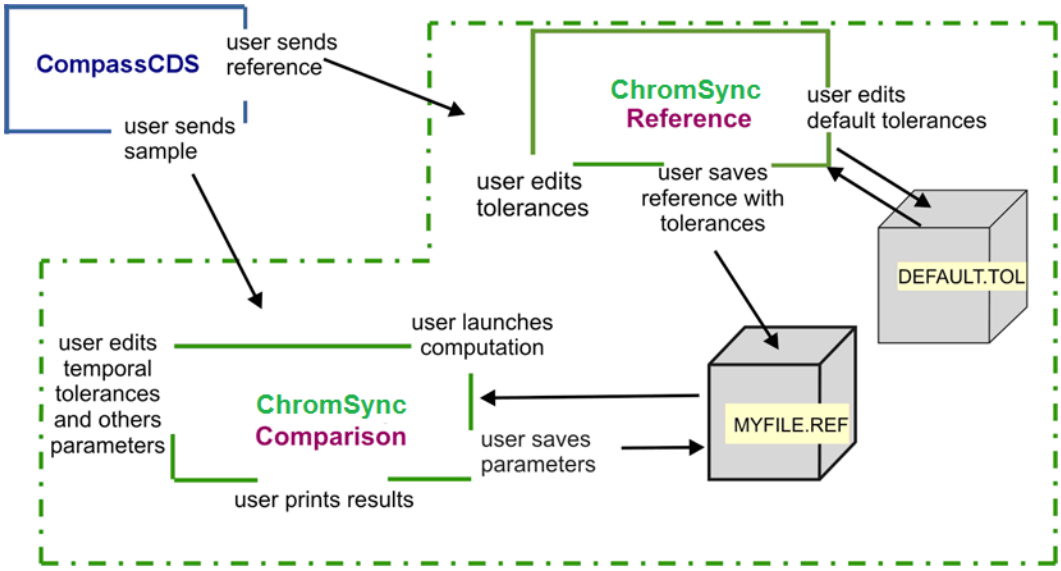
Installation

Insert the CompassCDS software media and choose Install Tools & Utilities. At the Install Add-ons page, choose ChromSync.

If the installation menu does not automatically load, navigate to the CD/DVD drive (usually D:) and select autorun.exe.

Getting started with CompassCDS ChromSync

Diagram of the application



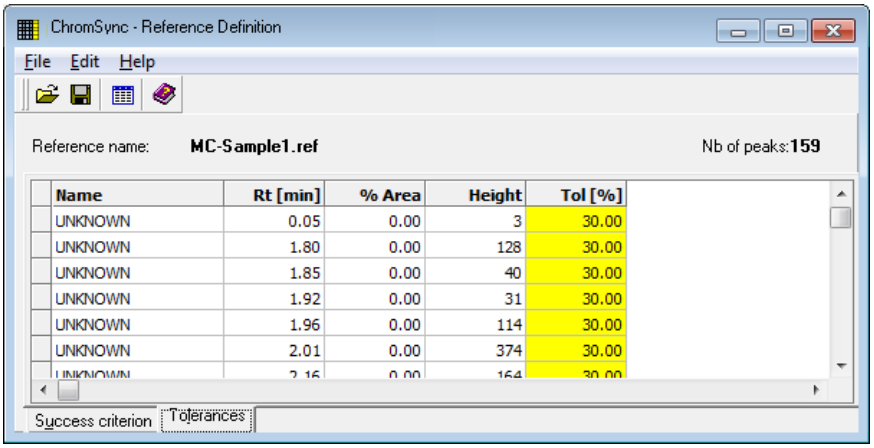
CompassCDS ChromSync is called from chromatography software: interactions between the user, CompassCDS and CompassCDS ChromSync.

CompassCDS ChromSync is called from the windows start menu or desktop: interactions between the user and CompassCDS ChromSync.

Using CompassCDS ChromSync Plug-in

Creating and saving a reference

Open the reference chromatogram. Select the *PLUG-INS / CHROMSYNC REFERENCE* menu. The following screen is displayed:


ChromSync - Reference Definition
File Edit Help
Reference name: MC-Sample1.ref
Nb of peaks:159
Name Rt [min] % Area Height Tol [%]
UNKNOWN 0.05 0.00 3 30.00
UNKNOWN 1.80 0.00 128 30.00
UNKNOWN 1.85 0.00 40 30.00
UNKNOWN 1.92 0.00 31 30.00
UNKNOWN 1.96 0.00 114 30.00
UNKNOWN 2.01 0.00 374 30.00
Success criterion
Tolerances

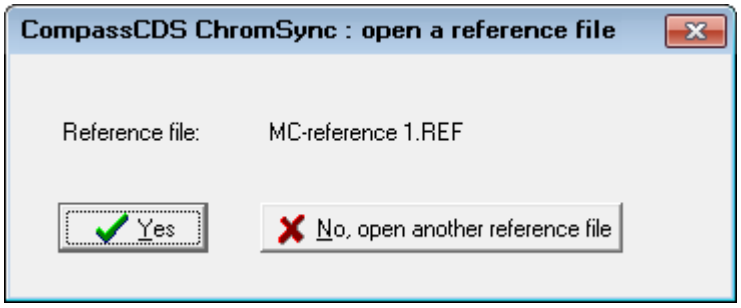
In the *Reference Name* field, the name of the selected chromatogram appears with the .REF extension. The number of peaks is also indicated.

- You can change the peak names by right clicking in the name column. Check the Edit peak names option. The Name column is displayed in yellow and you can modify the peak names.

- You can see and edit the theoretical indices (Kovatz) by selecting the Edit theoretical indices option. (Refer to the *Retention Indices* section for details).
- Press the button in the Reference Definition window or select the FILE / SAVE menu: the Save File window is displayed.
- In this screen, choose a name for the data file (for example: reference) and press the OK button.
- The reference chromatogram will be saved under filename.ref, with its tolerance parameters (Area %).

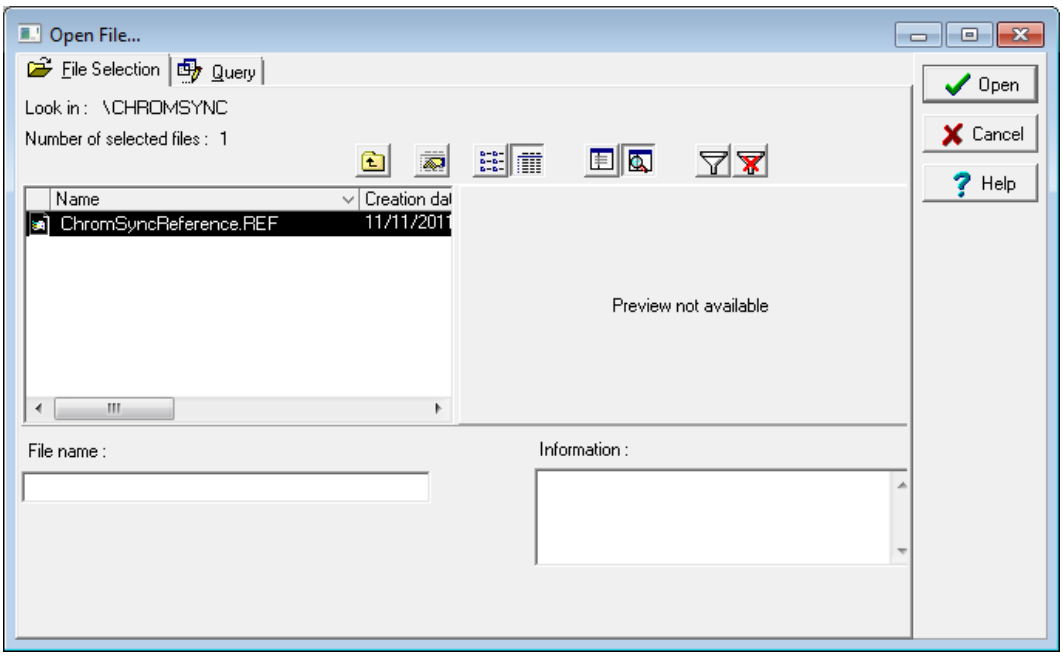
Comparison

Select the *PLUG-INS / CHROMSYNC COMPARE* menu. The following screen will appear if the reference directory is different.



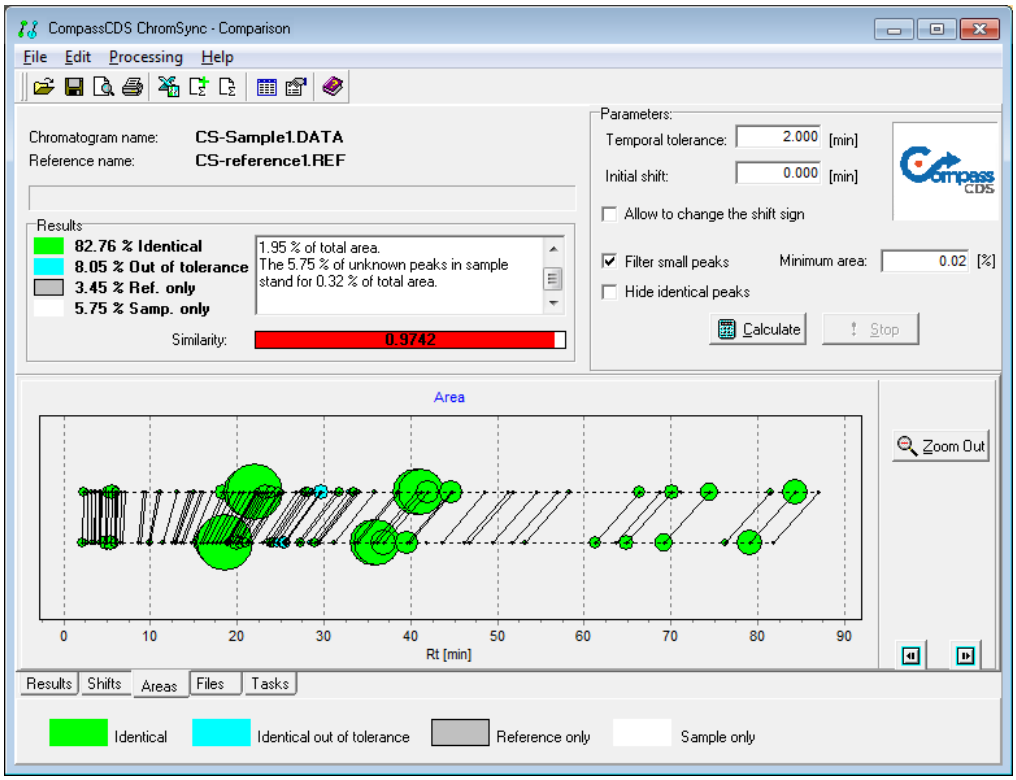
- Click on *YES* to choose this reference file.
- Click on *NO* to select another reference file.

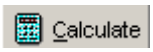
The following screen appears:



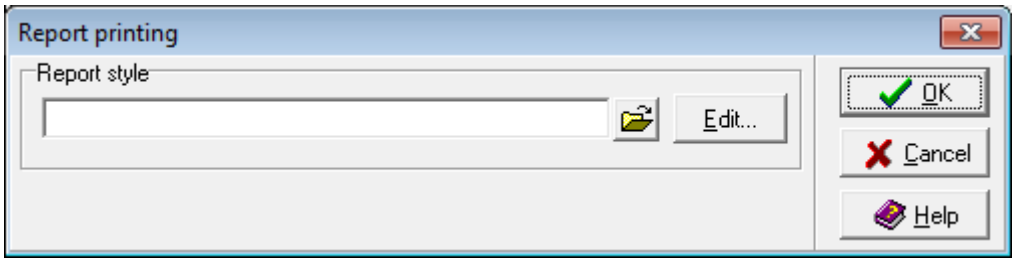
Select the new reference and click on *OK*.

- The comparison calculation is carried out and the comparison module is accessed.

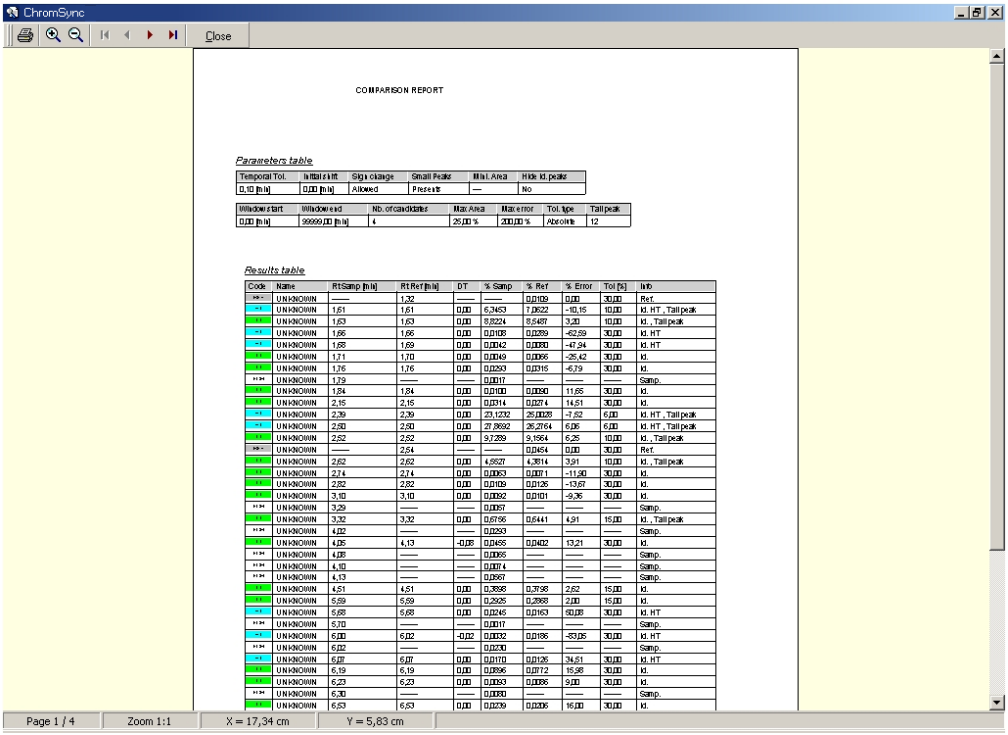


In the *Parameters* group, do not select the *Hide identical peaks* option. Click on  to compare the two chromatograms taking into account previous modifications. Identical peaks will match two comparison criteria: area and retention time. The area tolerance criterion defined in the reference file will also be verified. The peaks are represented by green disks.

If the matching is acceptable, and you wish to look at the final report, select the *FILE / PRINT PREVIEW* menu. The following screen is displayed:



When the required style is defined, click on *OK*. The following screen appears:



(This report is an example. Refer to the *Comparison Report* section to see how to create a report style.)

- Click on the button to print the comparison report

Details of the application

The different file types

The following files are accessible from CompassCDS ChromSync:

- Reference files with the .REF extension.
- AIA files with the .CDF extension.
- CompassCDS chromatograms with the .DATA extension.

AIA files (Analytical Instrument Association) used in chromatography contain several categories of information about the chromatogram:

- **Administrative information class:** operator name, experiment title, injection date and time, company method name, etc.
- **Sample description information class:** sample name, sample type, sample injection volume, sample amount, etc.
- **Detection method information class:** detection method comments, detection method name, detector name, detector maximum value, detector minimum value, detector unit, etc.
- **Raw data information class:** retention unit, sampling interval, etc.
- **Peak processing result information class**: peak number, peak processing method name, peak retention time, peak amount, peak start time, peak end time, peak width, peak area, peak area percent, peak height, peak asymmetry, peak efficiency, etc.

Most chromatography software can export data using the AIA format.

Choosing a Reference

How Can You Define a Reference?

A reference consists of four elements:

- a reference chromatogram,
- area tolerances on each peak of the reference chromatogram (refer to the *Area Tolerance* section),
- a success criterion (refer to the *Success Criterion* section),
- comparison parameters which indicate how to compare the reference chromatogram with the sample one. Associating these parameters values with the reference file is not required (refer to the *Matching* section).

All this information is saved in the .REF file; the first three via the Reference module and the last one via the Comparison module.

Area Tolerance

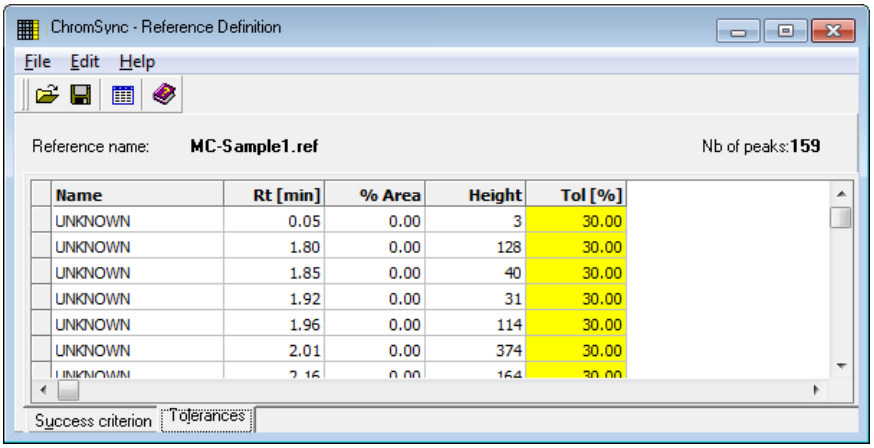
Definition

The area tolerance is defined in the Reference module and appears in the table located in the *Tolerances* tab (Tol [%] column).

The % Area criterion allows you to rapidly distinguish, with colors, the matched peaks verifying the tolerance percentage defined in the reference file. Two types of peaks can be thus found:

- “Identical” peaks: The area % error between the reference and the sample is inferior to the defined percentage (peaks displayed in green)
- "Out of tolerance" peaks: The area % error between the reference and the sample is superior to the defined percentage (peaks displayed in blue).

In both cases peaks are matched, which means that they verify the *temporal tolerance* and the *maximum error on area percentages* parameters (not to be confused with the tolerated area %).


ChromSync - Reference Definition
File Edit Help
Reference name: MC-Sample1.ref
Nb of peaks:159
Name Rt [min] % Area Height Tol [%]
UNKNOWN 0.05 0.00 3 30.00
UNKNOWN 1.80 0.00 128 30.00
UNKNOWN 1.85 0.00 40 30.00
UNKNOWN 1.92 0.00 31 30.00
UNKNOWN 1.96 0.00 114 30.00
UNKNOWN 2.01 0.00 374 30.00
Success criterion
Tolerances

This area tolerance (Tol [%]) is automatically given according to the size of the peak. It is however possible to change it separately. In most cases, the greater the peak area is, the smaller the tolerance is. The integration error for a small peak is much more significant than for a peak with a big area.

This tolerance criterion helps you to take into account area variations between the reference peaks and the sample peaks. With respect to this tolerance, a reference peak R and a sample peak S will match if the following area condition is present:

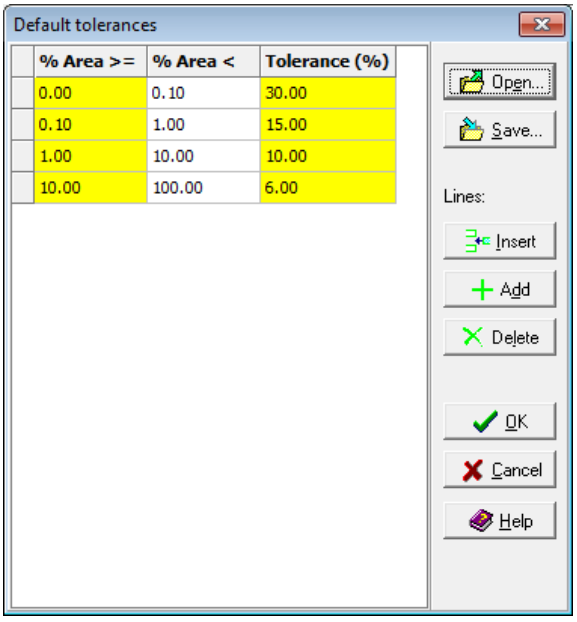
$$\frac{|\%Area(R) - \%Area(s)|}{\%Area(R)} \leq Tolerance(R) \quad \text{Where} \quad \%Area(peak) = \frac{Area(peak)}{TotalArea(chromatogram)}$$

If this tolerance criterion exceeds between matched peaks, the match is stamped "out of tolerance".

Setting the default tolerances

A default tolerance is assigned based on the size of the peak.

- To change these default values, choose the EDIT / *DEFAULT TOLERANCES* menu. The following window appears:



The default tolerance values are assigned for four area percentage levels. For example, in the table shown above, the peaks with areas between 1.00 and 10.00 percent of total area will be given a tolerance of 10 % of the expected area percentage.

- It is possible to change these default values. In the column named Tol (%), replace the actual value with a new one. To add, insert or delete area percentage level use the corresponding buttons. When you have added a new level, change the content of the column Area %>= and enter the minimum value of the % Area window.

- To accept the changes, press the

button. The default values will be updated in the Reference window: the former tolerance values (column Tol%) will be deleted.

- To save the values and in order to use them for other reference files, press the

button.

- The files saved in this screen can be opened with the

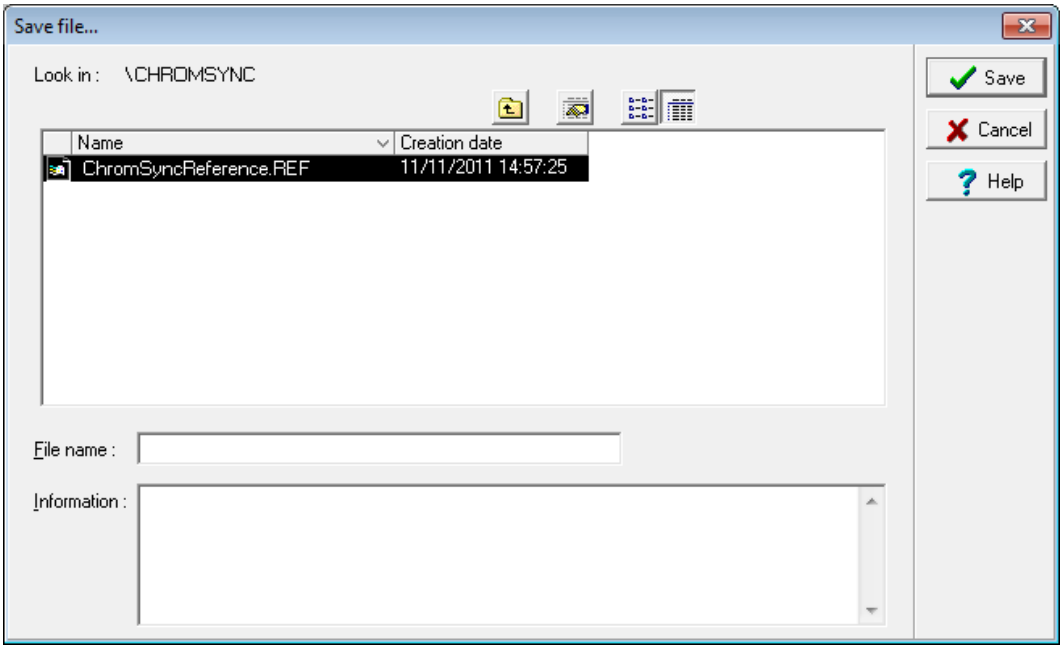
button.

How to open and save data

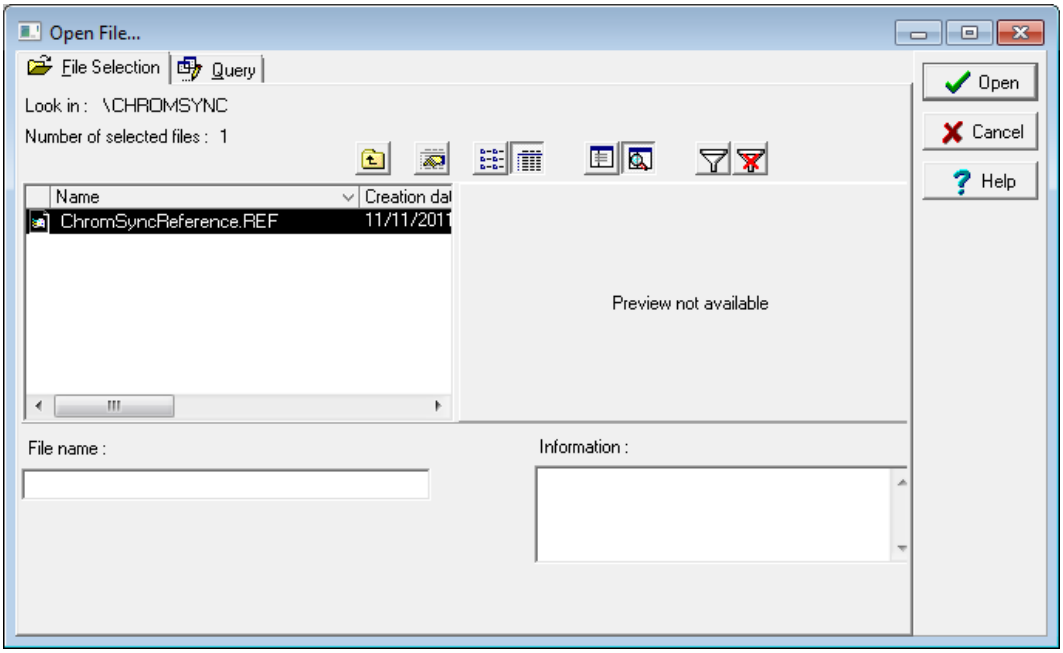
You must save the data. The program will ask for the name of the file in Comparison section of the software (to identify your reference chromatogram).

- When the reference parameters are acceptable, press , in the *Reference Definition* window, or choose the FILE / SAVE menu. Access the Save File window.

- In this window, choose a name for the reference file and press the *OK* button.



- To display previously saved data in the *Reference Definition* screen, press or choose the *FILE / OPEN* menu to open the *Open File* window.

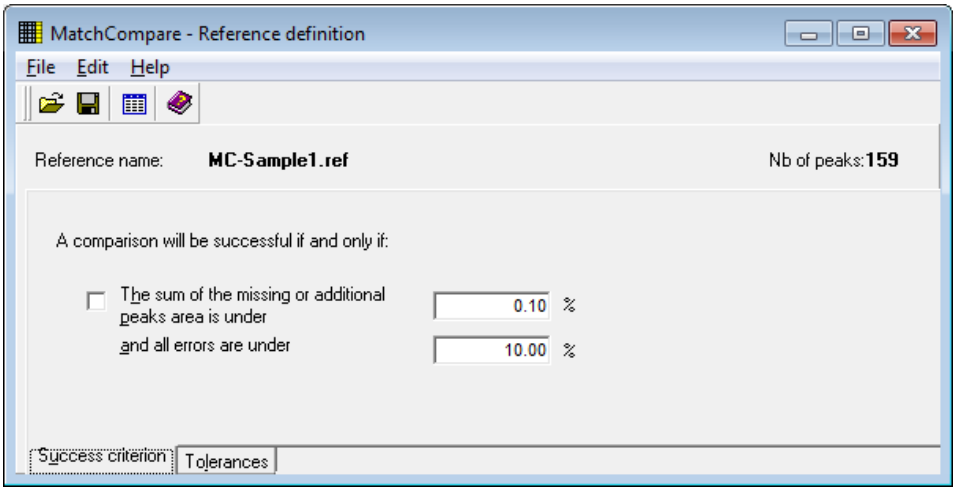


- Choose the name of the data file and press the *OK* button.

The Success Criterion

Success criterion is global. CompassCDS ChromSync only uses it at the end of the comparison.

To apply this criterion, select it in the *Success Criterion* tab of the *Reference Definition* window:


MatchCompare - Reference definition
File Edit Help
Reference name: MC-Sample1.ref
Nb of peaks:159
A comparison will be successful if and only if:
The sum of the missing or additional peaks area is under
0.10 %
and all errors are under
10.00 %
Success criterion
Tolerances

Two parameters are defined:

- Each area of additional and/or missing peaks in the sample chromatogram must be inferior to the first parameter.
- The second parameter corresponds to the error percentage between the sample chromatogram areas and the reference chromatogram areas. This error percentage must not be exceeded.

When these two parameters are attained, the comparison is successful.

Sample Choice and Processing

Choosing the Chromatograms to Compare

From Windows desktop: the sequence list

NOTE: You cannot use the sequence list if CompassCDS ChromSync is opened from CompassCDS.

Principle of the sequence list

CompassCDS ChromSync allows you to carry out a series of comparisons:

- It compares unknown chromatogram with different reference chromatograms
- It compares several unknown chromatograms with the same reference
- It compares unknown chromatograms with different references

Building a sequence list

Files can be located in the same directory or in different directories.

You must first create the reference files before performing the comparison. In the *Files* tab, select the reference chromatogram and click on the *Reference* button

or double-click on the chromatogram name; you access the *Reference Definition* window (refer to the *Reference* section). Save the reference.

Option 1: One reference with several sample chromatograms.

- In the *Files* tab, select the reference chromatogram (.REF extension) and the sample chromatograms to compare.

Remarks:

- When a file is selected, it appears back from the rest of the files .
- A book icon precedes reference files .
- A flask icon precedes sample files .

Click on the Compare button (

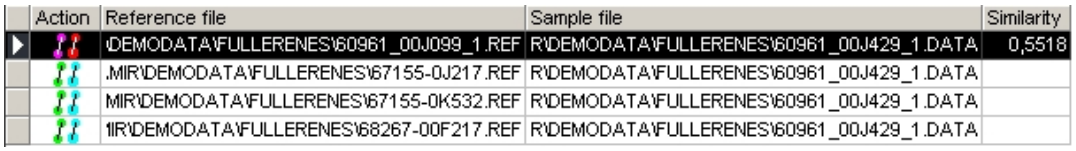
). This action generates:

- the building of the sequence list
- the first comparison of the sequence list which corresponds to the comparison between the reference and the sample chromatogram which was originally selected.

	Action	Reference file	Sample file	Similarity
▶		\DEMODATA\FULLERENES\60961_00J099_1.REF	:MODATA\FULLERENES\60961_00J429_1.DATA	0,5518
		\DEMODATA\FULLERENES\60961_00J099_1.REF	\IR\DEMODATA\FULLERENES\67155-0J217.CDF	

Option 2: Several references and one sample chromatogram.

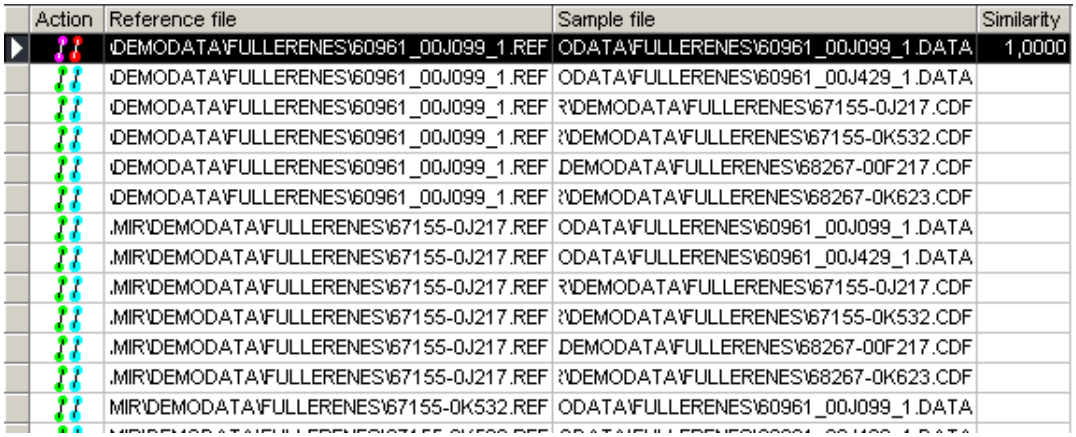
- In the *Files* tab, select the reference chromatograms and the sample chromatogram to compare with them.
- Select all references located in the same directory by right clicking and checking the *Select all references in the folder* option.
- If *Unselect all* option is selected, the program will cancel all the pre-selected files (in the same or different subdirectories). To cancel only one file, click on it.
- Click on the *Compare* button.



Action	Reference file	Sample file	Similarity
	\DEMODATA\FULLERENES\60961_00J099_1.REF	R\DEMODATA\FULLERENES\60961_00J429_1.DATA	0,5518
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	R\DEMODATA\FULLERENES\60961_00J429_1.DATA	
	MIR\DEMODATA\FULLERENES\67155-0K532.REF	R\DEMODATA\FULLERENES\60961_00J429_1.DATA	
	\IR\DEMODATA\FULLERENES\68267-00F217.REF	R\DEMODATA\FULLERENES\60961_00J429_1.DATA	

Option 3: Several reference chromatograms and several samples.

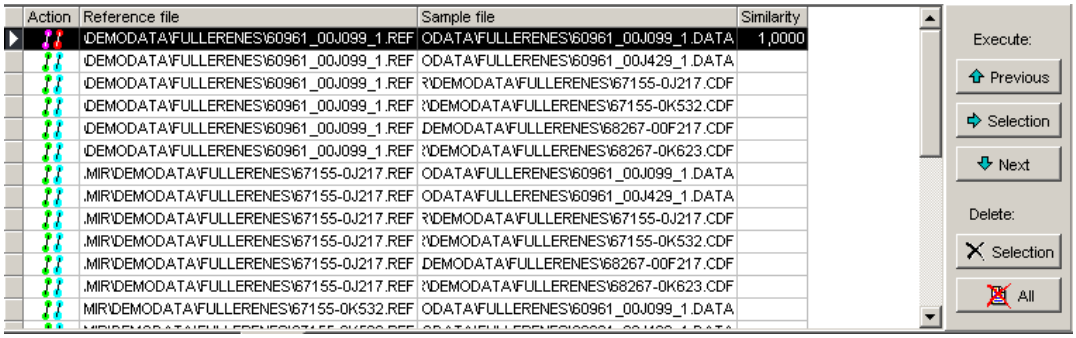
- In the Files tab, select the reference and sample chromatograms.
- Click on the Compare button: CompassCDS ChromSync will display all possible comparison combinations.



Action	Reference file	Sample file	Similarity
	\DEMODATA\FULLERENES\60961_00J099_1.REF	ODATA\FULLERENES\60961_00J099_1.DATA	1,0000
	\DEMODATA\FULLERENES\60961_00J099_1.REF	ODATA\FULLERENES\60961_00J429_1.DATA	
	\DEMODATA\FULLERENES\60961_00J099_1.REF	R\DEMODATA\FULLERENES\67155-0J217.CDF	
	\DEMODATA\FULLERENES\60961_00J099_1.REF	R\DEMODATA\FULLERENES\67155-0K532.CDF	
	\DEMODATA\FULLERENES\60961_00J099_1.REF	DEMODATA\FULLERENES\68267-00F217.CDF	
	\DEMODATA\FULLERENES\60961_00J099_1.REF	R\DEMODATA\FULLERENES\68267-0K623.CDF	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	ODATA\FULLERENES\60961_00J099_1.DATA	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	ODATA\FULLERENES\60961_00J429_1.DATA	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	R\DEMODATA\FULLERENES\67155-0J217.CDF	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	R\DEMODATA\FULLERENES\67155-0K532.CDF	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	DEMODATA\FULLERENES\68267-00F217.CDF	
	.MIR\DEMODATA\FULLERENES\67155-0J217.REF	R\DEMODATA\FULLERENES\68267-0K623.CDF	
	MIR\DEMODATA\FULLERENES\67155-0K532.REF	ODATA\FULLERENES\60961_00J099_1.DATA	

When the disk content has changed, update it by clicking on the *Update* button.

Running the sequence list



The sequence list contains the following information:

Action: Setting a reference is identified by the icon.

Comparison between two chromatograms is identified by the icon.

Reference file: name and data path of the reference chromatogram

Sample file: name and data path of the sample chromatogram

Similarity: result of the similarity calculation

: to perform the action corresponding to the selected line. A double click on the current line gives the same result.

: to perform the action corresponding to the preceding line.

: to perform the action corresponding to the next line.

The three tabs *Results*, *Shifts,* and *Areas* always display the results associated with the last comparison.

: to delete the selected line.

: to delete the entire sequence list.

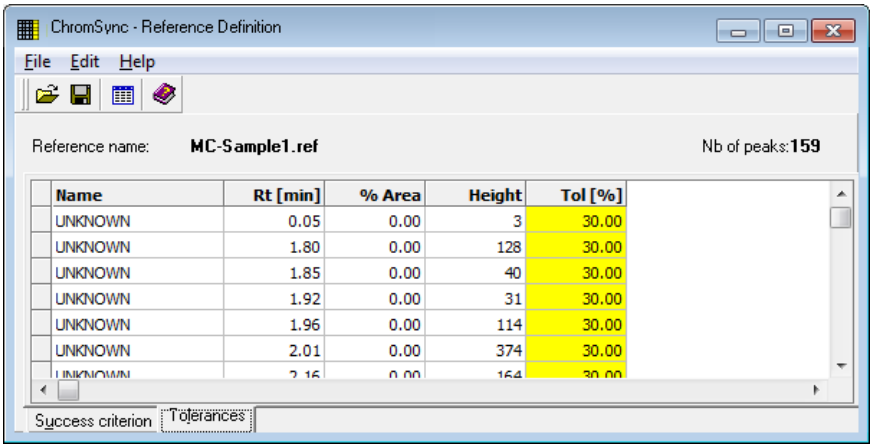
Using ChromSync Plug-in within CompassCDS

A CompassCDS plug-in is a program using a .dll file which is opened from CompassCDS in post-run or in direct call. The goal of this program is to execute a free processing not included in the standard chromatography software.

Using the Plug-in in direct call

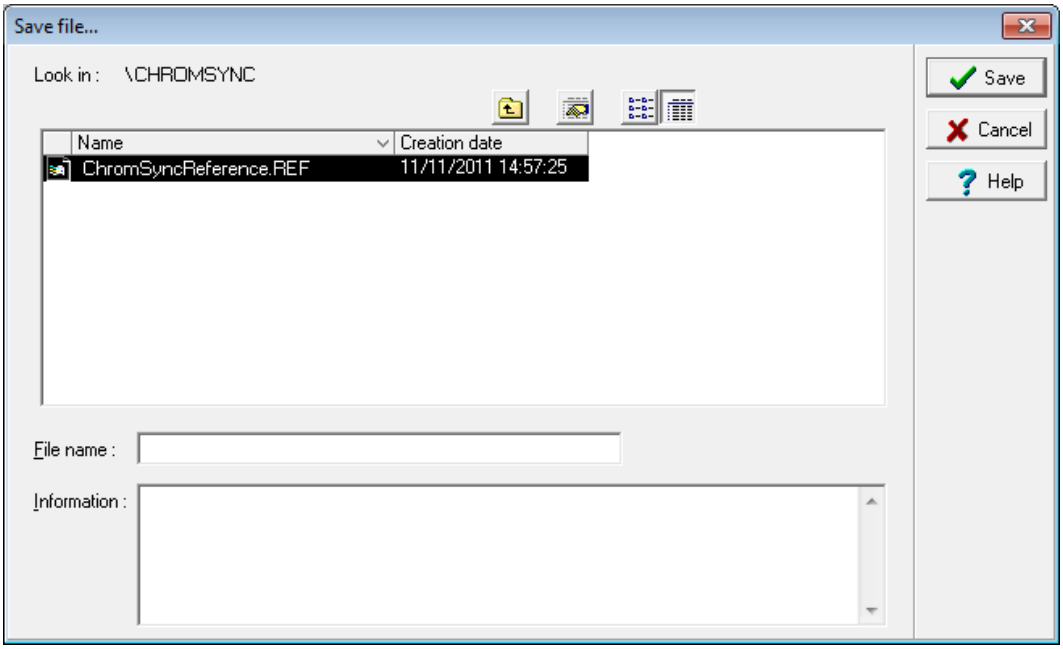
This function enables the Plug-in as an interactive mode to create the reference files.

- Open the chromatogram. Select the *PLUG-INS / CHROMSYNC REFERENCE* menu; the following screen is displayed.


ChromSync - Reference Definition
File Edit Help
Reference name: MC-Sample1.ref
Nb of peaks:159
Name Rt [min] % Area Height Tol [%]
UNKNOWN 0.05 0.00 3 30.00
UNKNOWN 1.80 0.00 128 30.00
UNKNOWN 1.85 0.00 40 30.00
UNKNOWN 1.92 0.00 31 30.00
UNKNOWN 1.96 0.00 114 30.00
UNKNOWN 2.01 0.00 374 30.00
Success criterion
Tolerances

Save the reference with the button or the *FILE / SAVE* menu.

The following screen appears:

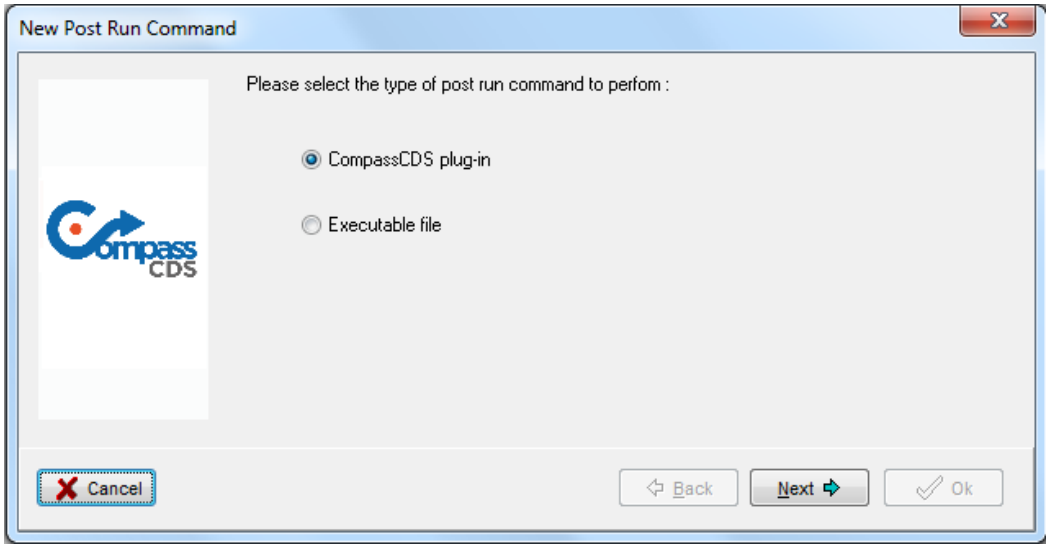


Open the sample chromatogram to be compared and select the *PLUG-INS / CHROMSYNC COMPARE* menu. The sample is compared to the last computed reference.

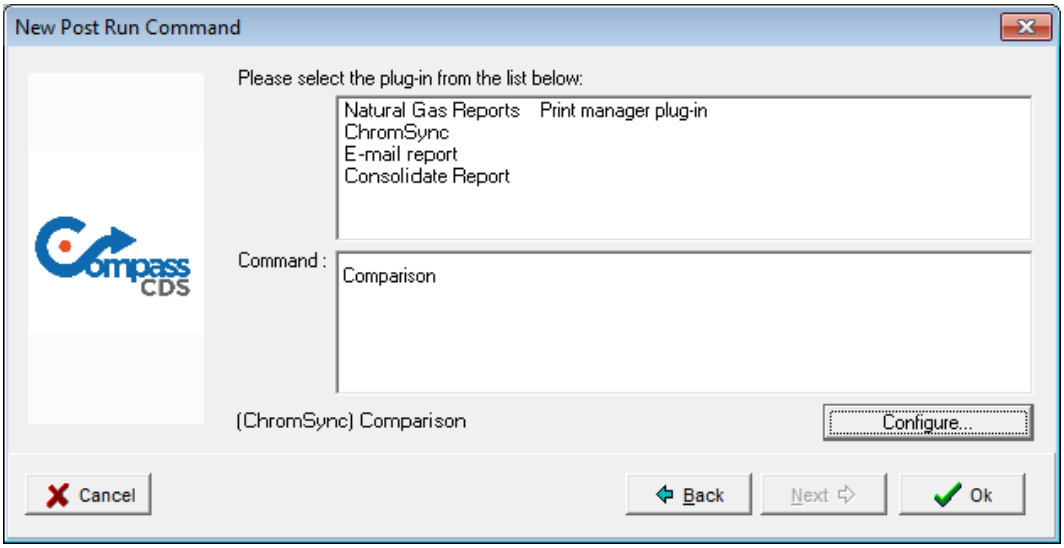
Using the Plug-in in post-run

If you want to execute a comparison calculation at the end of each acquisition, you need to insert the Plug-in in the method.

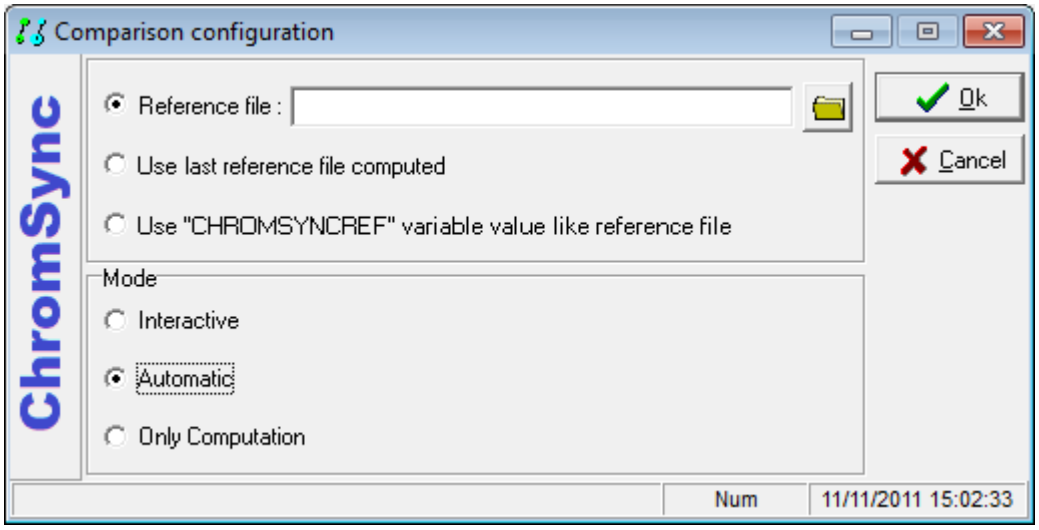
- In the post-processing phase of the method, press Add... and select the CompassCDS Plug-in option then press Next >>.



- In the following step, choose ChromSync Plug-in and press Next >>.
- In the following screen, press Configure...



The following window appears:



- Check the *Reference file* option and press the button to manually select the reference chromatogram.
- Check the *Use last reference file computed* option to use the last reference in memory.
- Check the *Use "MATCHREF" variable value like reference file* option when the reference filename is given by this variable.

To use this option, you have to create the MATCHREF variable (identifier) in the method variable editor. This variable is a global user input variable. The user must enter the complete name of the reference file (filename.REF) in the user input field when starting a single acquisition or a sequence (refer to the *CompassCDS Chromatography Data System* manual).

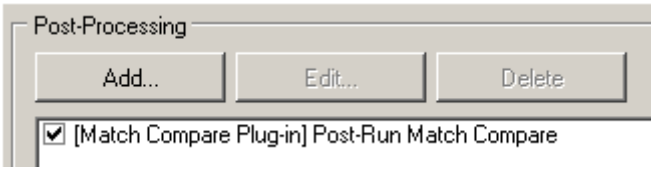
- Choose the computing *mode*:

Interactive: the *ChromSync Comparison* window will be automatically displayed for each processing and will allow user to change the comparison parameters and decide whether or not to print the comparison report.

Automatic: the *ChromSync Comparison* window is not displayed and a comparison report is automatically printed at the end of each processing.

Only Computation: the *ChromSync Comparison* window is not displayed and no comparison report is automatically printed at the end of each processing.

- When all parameters have been defined, click on *OK* button.
- Press the button: a new line is added in the post-processing section of the method :



- You can edit the Plug-in to change some parameters :
- Run Match Compare line and press the button.
- To delete the Plug-in : click on the Post-Run Match Compare line and press the button.

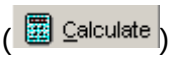
Matching

Matching Parameters

The main matching parameters are the *temporal tolerance*, defined in the standard parameters page, and the *Max. Error* parameter, defined in the advanced parameters page. In most of the matchings, both criteria are verified. But in some rare cases, the matching is done without the temporal tolerance parameter being verified. CompassCDS ChromSync estimates that the peaks are comparable.

The calculation for temporal tolerance is defined in the *Standard Comparison Parameters* chapter. The rejection area determines the maximum area difference authorized between a reference peak and a sample one.

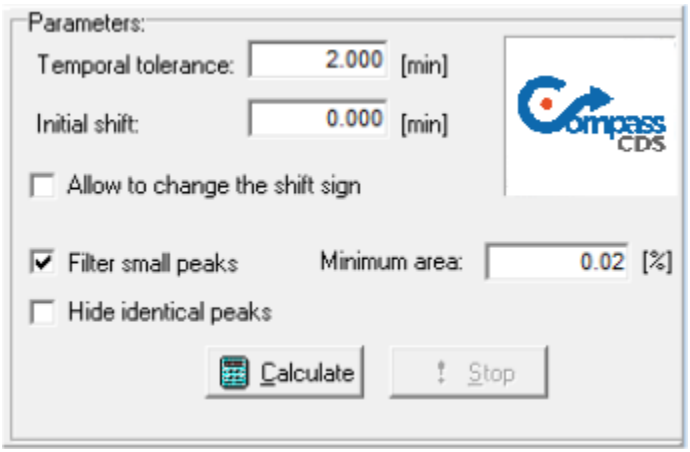
Setting the comparison parameters

When you change the comparison parameters, remember to update the results with the *Calculate* button () or select the *PROCESSING / CALCULATE* menu.

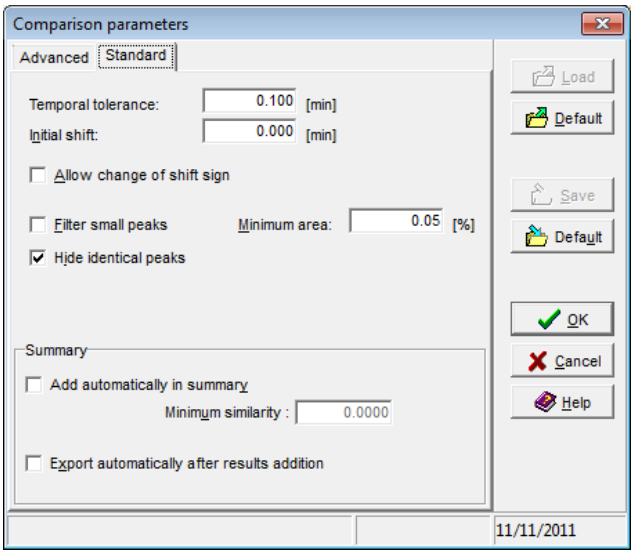
In some particular situations (difficult comparison), the calculation time can be important: press the button or select the *PROCESSING / STOP* menu, to stop calculations and to define other comparison parameters.

Standard comparison parameters

These parameters can be modified in the main window of the CompassCDS ChromSync Comparison module.



Users can also modify the parameters by selecting the *EDIT* / *PARAMETERS* / *STANDARD* menu or by clicking on the icon.



The following parameters have a direct influence on the matching:

- **Temporal Tolerance**: the temporal tolerance defines a period of time around the reference retention time corrected by the average shift. With respect to this average shift and the temporal tolerance, a reference peak R whose retention time is Tr and a sample peak S whose retention time is Ts will match if:

$$\left|\mathrm{Ts} - \mathrm{Tr} - \text{average shift}\right| \leq \text{Temporal tolerance}$$

The average shift is calculated over the 3 previous peaks shift.

If necessary, CompassCDS ChromSync may accept a match between two peaks even when the condition above is not verified. This match is called “out of temporal tolerance”.

Most of the matches can be successfully realized with a temporal tolerance between 0.05 and 0.2 min. For some particular comparison, you can choose an important temporal tolerance but the algorithm may accept erroneous matches.

See also advanced comparison parameters for the choice of relative or absolute temporal tolerance.

- **The Initial Shift:** the default value equals zero, however it is possible to set an initial shift, if the two chromatograms have not been recorded at the same time. The initial shift can be useful to reduce temporal tolerance and to limit comparison mistakes.

- **The Allow change of shift sign option:** if this check box is not selected, the shift is allowed to vary only one way. In other words, if the first peak is late, all the peaks have to be late or they will not be considered to match. If the first peak is ahead, all the peaks have to be ahead or they will not be considered to match. So the *Allow change of shift sign* option should be selected when the shift oscillates around 0.0.

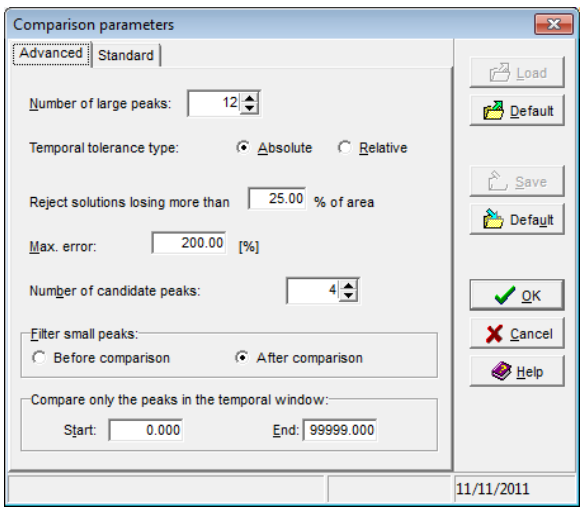
- **The choice of including or not small peaks:** if this check box is selected, small peaks whose areas are lower than the specified value (*minimum area*) will be excluded from the calculations, if they do not match. Filtering is realized at the end of comparison thus small peaks are considered during calculation. This parameter is important for the final comparison report.

See also advanced comparison parameters for the possibility to filter small peaks before or after the comparison.

- **The choice of hiding or not identical correct peaks**: if this check box is checked, the peaks respecting the two tolerance criteria (peaks displayed in green) will not be displayed in the diagram. This option can be interesting to point out all the peaks which are not coupled, essentially if chromatograms are dense.

Advanced comparison parameters

Users can access these parameters by selecting the *EDIT / PARAMETERS / ADVANCED* menu.



The number of large peaks (Default value: 12): this criterion is useful in reducing calculation time. In this case, the comparison is performed in two steps:

- Given a number of large peaks n, defined by the user. CompassCDS ChromSync first compares the n larger peaks of the reference chromatogram with the sample ones (in area percentages).

- Next, the comparison algorithm is performed in each zone determined in the previous step.

The choice of Relative or Absolute temporal tolerance:

When *Absolute temporal tolerance* is selected, the size of the zone is constant for all peaks. The temporal condition becomes:

$$\left|\mathrm{Ts} - \mathrm{Tr} - \text{average shift}\right| \leq \text{Absolute temporal tolerance}$$

When *Relative temporal tolerance* is selected, the size of the zone increases linearly with the retention time of the reference peaks. The temporal condition to respect becomes:

$$\left|\frac{\mathrm{Ts} - \mathrm{Tr} - \text{average shift}}{\mathrm{Ts}}\right| \times 100 \leq \text{Relative temporal tolerance}$$

Usually, the absolute mode will be used for comparison. The relative mode can be used to compare chromatograms where a temporal shift (evolving according time) appears during analysis.

NOTE: When temporal tolerance is too high, the calculation time can become critical.

- **Number of** candidate peaks (Default value: 4): determines the number of peaks in the sample chromatogram that CompassCDS ChromSync matches against a given reference peak. This parameter allows users to minimize the influence of a large temporal tolerance. When the temporal tolerance is increased, it may be necessary to increase the number of sample peaks (10 for example). However, keep in mind that the erroneous match risk is increased too.

NOTE: When the number is too high, the calculation time can become critical.

The choice of reject solutions (Default value: 25%): all the solutions losing more than the specified percentage of area (area of the reference plus area of the sample) are rejected by CompassCDS ChromSync.

A loss of area occurs when a peak is not matched. If this parameter is too high, CompassCDS ChromSync will consider a larger number of matches. But CompassCDS ChromSync can also decide to isolate a peak with a relatively great area, which is not mandatory the good solution. This parameter can be increased to reject a critical sample peak, if it is not present in the reference.

- **The maximum error (Default value: 200%):** if the area difference between a sample peak and a reference peak is greater than the default, CompassCDS ChromSync will reject the match.

In most cases if matches are out of tolerance, the error does not exceed 100%. Yet, when some concentration problems occur, you may need to increase this parameter. For example, a small peak which is expected at 0.05% (according to the reference) can have a higher area percentage (0.3%, because of the total area). The error is then 500%.

- **Filter small peaks** (Default value: after comparison): when the *Before Comparison* option is selected, small peaks whose areas area inferior to the minimum area are deleted before the comparison calculation. This option is useful for difficult comparison. If the *After Comparison* option is selected, non-matching small peaks are removed after the comparison calculation. This option allows you to delete small peaks in the results displayed.

- **The temporal window for comparison**: this parameter is used to define a temporal window where only the peaks present in this window are used for the comparison.

Most of the comparisons can be performed with the default values assigned to two categories of parameters:

Standard parameters:

Temporal tolerance: 0.100 min

Initial shift: 0.000 min

Allow change of shift sign: not checked

Filter small peaks: minimum area 0.05% when this option is checked

Hide identical peaks: checked

Advanced parameters:

Number of large peaks: 12

Temporal tolerance type: absolute

Reject solutions losing more than 25% of area

Max. error: 200%

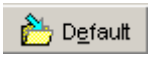
Number of candidate peaks: 4

Filter small peaks after comparison

Changing the Default Values

When default values for the comparison parameters are not correct, you can set your own default values in the *Comparison Parameters* window and save them as default values, so that when you open the comparison module, these values are loaded.

You can associate these parameter values to the reference file in order to create comparison methods.

- To save the parameters as default values, for the current user, press the 

button, in the *Comparison Parameters* window.
- To load the default parameters, press the

button.
- To save the parameters in the reference file (and create a comparison method associated to the reference), press the

button.
- To load saved parameters, press the

button.

Some details about the comparison algorithm

CompassCDS ChromSync will attempt to satisfy the criteria defined by the user. However, it also uses special techniques to determine a correct match. In this case, CompassCDS ChromSync may reject a match between two peaks based on user criteria. Two peaks that do not match as defined by user criteria may be considered as matched by CompassCDS ChromSync. This feature of CompassCDS ChromSync helps you identify peaks that match out of tolerance.

For example, if a peak seems to match, but involves a significant change in the shift that is not confirmed by the following peaks, this peak will not be considered to match. If a peak does not match because its shift is too large, but the shift of the following matching peaks is similar, the peak will be considered to match.

The accuracy of processing is based on tolerance criteria. CompassCDS ChromSync will attempt to correct the chromatogram defaults.

CompassCDS ChromSync calculates a parameter called *similarity* between the reference and the sample chromatograms. This similarity is a weighted average of the values M1 and M2 as presented below:

M1 concerns the ratio of matching peaks:

$$M1 = \frac{2 \times NumberOfMatchingPeaks}{NumberOfPeaks(SampleChrom.) + NumberOfPeaks(ReferenceChrom)}$$

M2 concerns the ratio of “matching area” (areas of matching peaks):

$$M2 = \sum_{p=1}^{NumberOfMatchingPeaks} \frac{Area(SamplePeak_p) + Area(ReferencePeak_p)}{ToralArea(SampleChrom) + TotalArea(ReferenceChrom)}$$

The similarity is a weighted mean between M1 and M2:

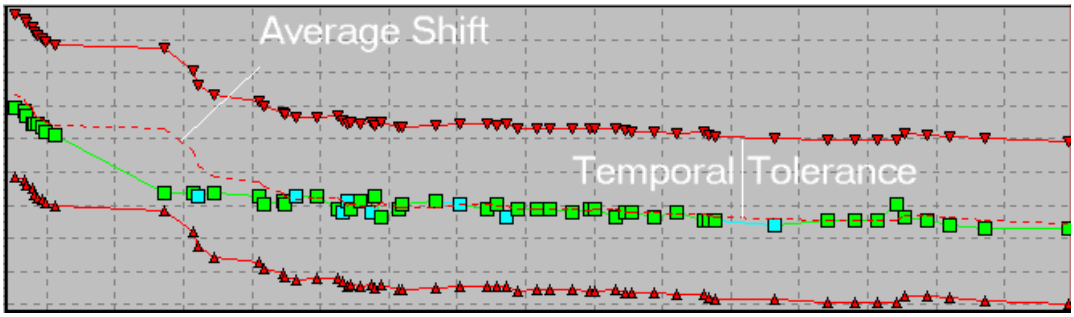
$$M = \alpha \times M1 + \beta \times M2$$
$$\alpha = 0.95; \beta = 0.05$$

Displaying the Results

CompassCDS ChromSync offers three ways of displaying the comparison results.

The Time Shift

The shift (*Shifts* tab) is the difference between the retention time of the reference peaks and the sample peaks. The shift must be similar from one peak to the next peak. If it is significantly different (over than the temporal tolerance) the peaks may match. In this case, an average shift is calculated and updated for each new matching peak, as shown on the following graph:



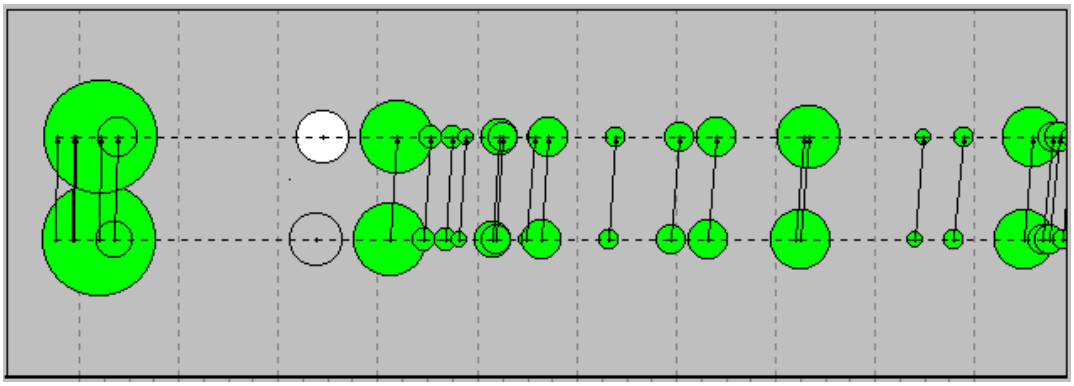
This graph shows the time shift versus reference retention time.

Small triangles are displayed for each reference peak to show the temporal tolerance zone for each reference peak. A triangle shows the lowest bound of this zone while an up-bottom triangle shows the upper bound. Inside this zone a small square, which corresponds to the sample peak matched with the current reference peak, is usually displayed. As a reference peak may have no matching sample peak, there may be no square inside a temporal tolerance zone.

NOTE: As noted in the introduction, CompassCDS ChromSync may match two peaks without respect for the temporal tolerance criterion. The only way to identify it as a match is to view the previous graph. I this case, the squares representing the matching peaks, which do not verify this criterion, will be outside of the interval defined by the triangles representing the temporal tolerance.

Peak Areas

CompassCDS ChromSync represents each peak by colored disk (*Areas* tab). Each disk area is proportional to the corresponding peak area and the disks are centered on the retention time of peaks. The upper disks correspond to the sample chromatogram while the lower disks correspond to the reference chromatogram.



When you put the cursor on the center of the disk, the area percentage and the retention time of the corresponding peak are displayed on the right side of the window.

The color gives information about the Area % tolerance criterion (defined in the reference).

Zoom function:

- Zoom-in by first selecting the upper-left point of the rectangle, then clicking and dragging with the left mouse button. A zoom-out is obtained by selecting first the lower-right point, or by clicking the *Zoom out* button:

.

- You can pan across the graph by pressing the right mouse button.

In the *Areas* tab, you can also pan across the graph by pressing the following buttons (the scrolling speed will increase progressively):

- : to scroll from right to left
- : to scroll from left to right.

Results Peak by Peak

Results are displayed peak by peak in the *Results* tab. The results are shown by pair if a sample peak matched with a reference peak. If some cells are empty, the given results may reference a peak that could not be matched.

Name	Rt Samp [min]	Rt Ref [min]	DT	% Samp	% Ref	% Error	Tol [%]	Info
Unknown	3,89	3,84	0,05	0,8011	0,7734	3,58	15,00	
Unknown	4,75	4,67	0,08	4,3107	4,1168	4,71	10,00	
Unknown	4,85	4,77	0,08	0,8131	0,9922	-18,05	15,00	
Unknown	6,13	6,00	0,13	24,6972	24,9366	-0,96	6,00	pass 1
Unknown	6,93	6,79	0,14	2,8976	2,6479	9,43	10,00	
Unknown	17,26	------	------	5,5448	------	0,00	100,00	
Unknown	------	16,94	------	------	5,5669	0,00	10,00	
Unknown	20,96	20,62	0,34	10,1629	10,1660	-0,03	6,00	pass 1
Unknown	22,67	22,31	0,36	1,0807	1,0788	0,17	10,00	
Unknown	23,78	23,44	0,34	1,0559	1,0798	-2,22	10,00	
Unknown	24,43	24,07	0,36	0,5833	0,6092	-4,24	15,00	

Name: name of the reference peaks.

Rt Samp [min]: retention time of the sample peak.

Rt Ref [min]: retention time of the reference peak.

ΔT: difference between the retention times.

% Samp: area percentage of the sample peak.

% Ref: area percentage of the reference peak.

% Error: the error in percent between the area of the sample peak and the reference one.

If this percent error is lower than the area percentage tolerance (next column), peaks are called identical (green) otherwise it is 'out of tolerance' (blue).

Tol [%]: area percentage tolerance, defined for each reference peak in the Reference module.

Information: results of the comparison with the user parameters.

Remarks: user editable field.

Index 1: first index which comes from the reference file.

Index 2: second index which comes from the reference file.

Ref Index: Kovats index of the reference file.

Sample Index: Kovats index of the sample file.

Global Estimate of the Comparison

In the *Results* area, you can see an estimate of the comparison:

The first part concerns the percentages of matching or not matching peaks.

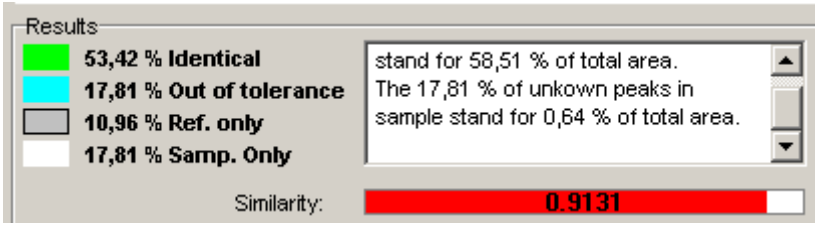
% Identical: gives % of matching peaks (respecting the two criteria) and verifying the % Area tolerance.

% Out of tolerance: gives % of matching peaks that exceeds the % Area tolerance parameter.

% Ref. only: gives the number of peaks present only in the reference divided by the total number of peaks.

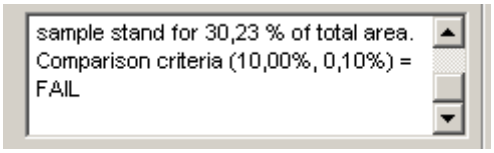
% Samp. only: gives the number of peaks present only in the sample divided by the total number of peaks.

The total number of peaks represents the number of matching peaks plus the number of peaks present only in the reference, plus the number of peaks present only in the sample.

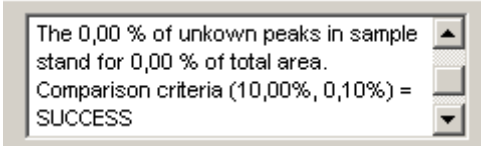

Results
53,42 % Identical
17,81 % Out of tolerance
10,96 % Ref. only
17,81 % Samp. Only
stand for 58,51 % of total area.
The 17,81 % of unkown peaks in
sample stand for 0,64 % of total area.
Similarity:
0.9131

If success criteria have been specified the comparison result appears as follows:

FAIL is displayed if the comparison does not match the success criterion:



PASS is displayed if the comparison matches this criterion:



The specified comparison criteria are put into brackets.

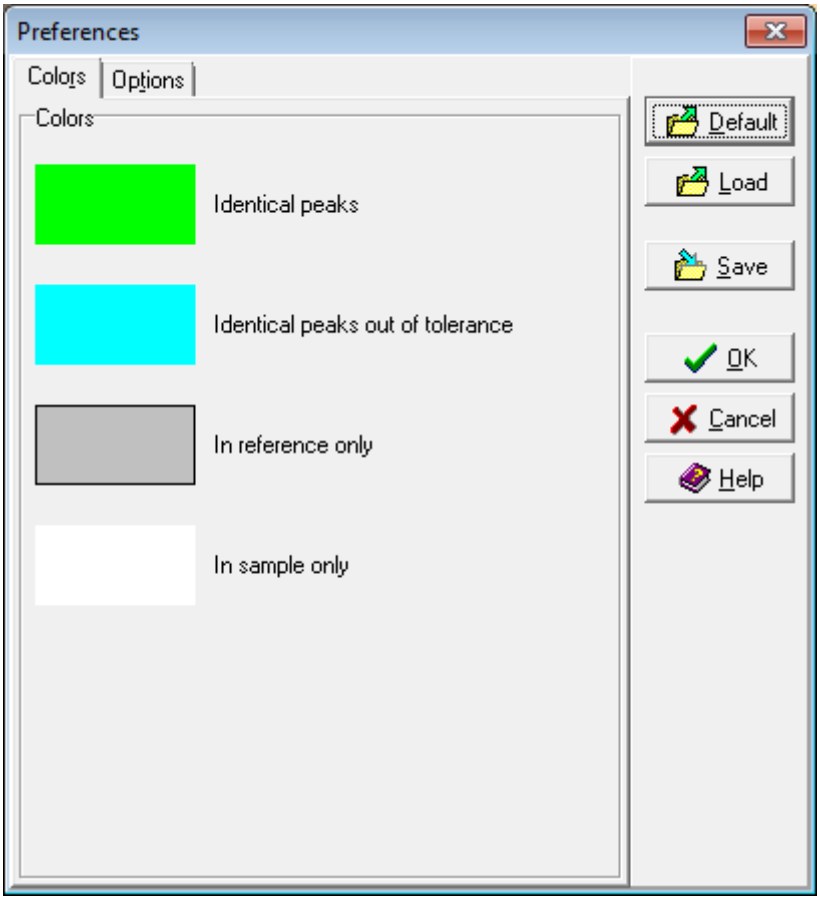
- CompassCDS ChromSync also computes a *similarity* measure between reference and sample chromatograms.

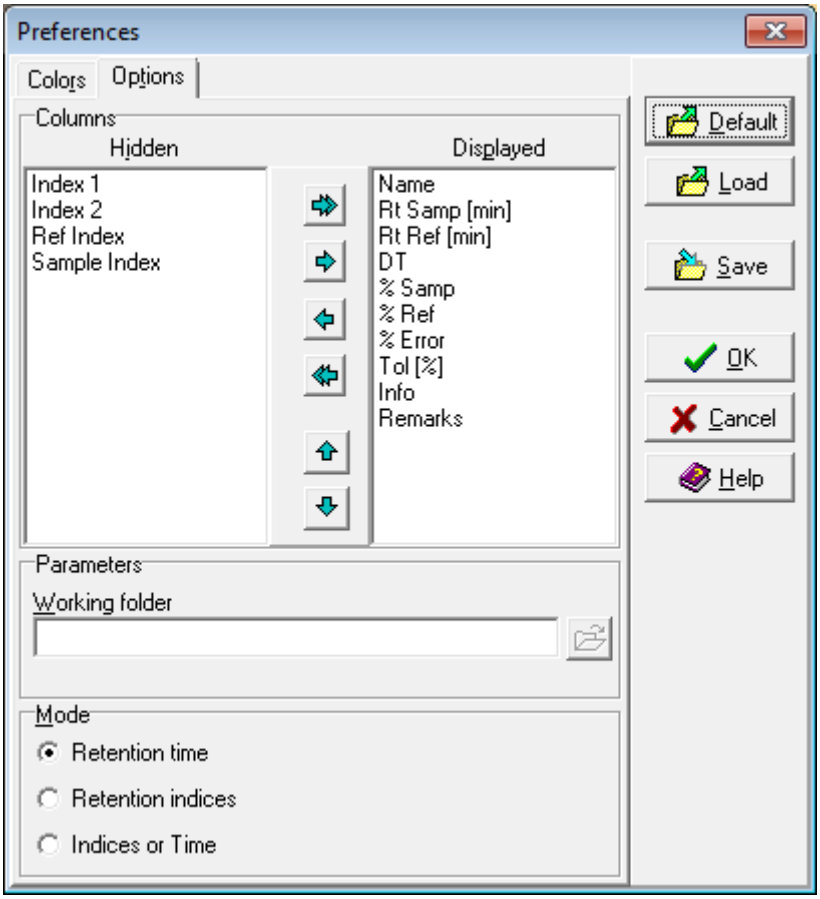
Modifying the Result Display

To display the *Preferences* window, select the *EDIT / PREFERENCES* menu or click on the button.

Preferences Description

The *Preferences* window contains two tabs: Colors and Options.





The preference window allows you to modify results color, to customize the printout and displayed columns and to specify the calculation mode (indices or retention times).

Color modification affects time shifts, area curves, and results table displays (respectively *Shifts*, *Areas*, *Results* tabs). Column customization only affects the results tables display (*Results* tab), printed reports, and Excel reports.

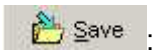
Colors tab

Matching and non-matching are represented by the following colors:

Identical peaks	**Identical**	→ **Green**
Identical peaks out of tolerance	**Identical out of tolerance**	→ **Blue**
In reference only	**Only in the reference**	→ **Grey**
In sample only	**Only in the sample**	→ **White**

The *Colors* tab contains the following buttons:

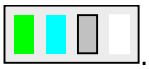
: To return to default values



: To save the modifications

: To load the last saved preferences

Usual buttons as OK, Cancel, Help.

To change default colors, click on the colored rectangle of interest  ..

Modified rectangles appear as follows:

Save the modifications by clicking on the *Save* button (

).

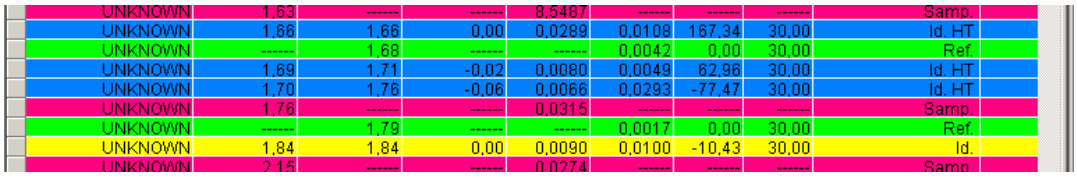
The *Load* button becomes active (

).

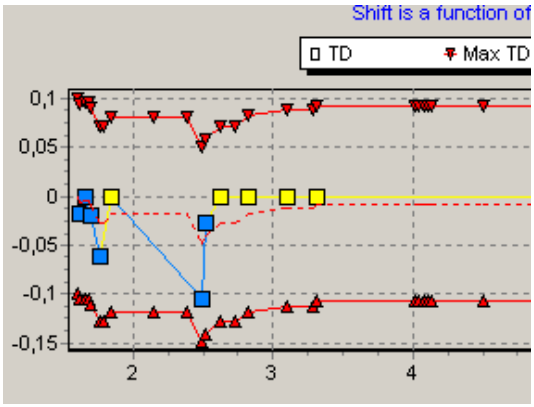
When all modifications are completed in the module, validate by *OK*.

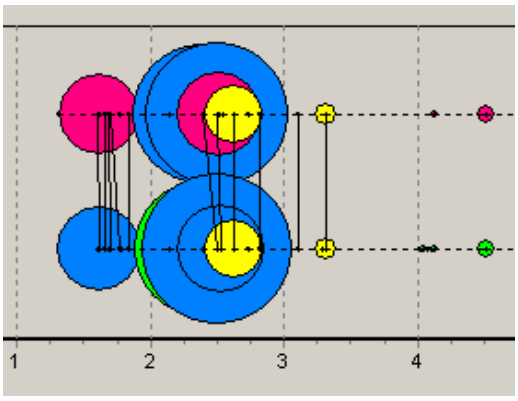
The modifications are applied in the following areas of the application:

- In the *Results* tab



- In the Shifts and Areas tabs



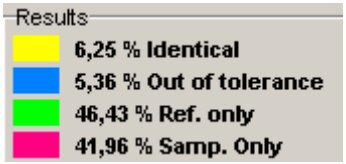


- In the comparison report (Print preview)

Code	Name	RtSamp [min]	RtRef [min]	DT	% Samp	% Ref	% Error	Tol [%]	Info
	UNKNOWN	—	6,23	—	—	0,0093	0,00	30,00	Ref.
	UNKNOWN	—	6,30	—	—	0,0080	0,00	30,00	Ref.
	UNKNOWN	—	6,53	—	—	0,0239	0,00	30,00	Ref.
	UNKNOWN	—	6,55	—	—	0,0168	0,00	30,00	Ref.
	UNKNOWN	—	6,57	—	—	0,0096	0,00	30,00	Ref.
	UNKNOWN	—	6,64	—	—	0,0126	0,00	30,00	Ref.
	UNKNOWN	—	6,75	—	—	0,0130	0,00	30,00	Ref.
	UNKNOWN	—	6,76	—	—	0,0190	0,00	30,00	Ref.
	UNKNOWN	—	7,07	—	—	0,4682	0,00	15,00	Ref.
	UNKNOWN	7,08	7,08	0,00	0,4524	0,4694	-3,61	15,00	Id., Tall peak
	UNKNOWN	7,12	7,12	0,00	5,8732	5,7966	1,32	10,00	Id., Tall peak
	UNKNOWN	7,21	—	—	0,0476	—	—	—	Samp.
	UNKNOWN	7,23	—	—	0,0098	—	—	—	Samp.
	UNKNOWN	7,28	—	—	8,9073	—	—	—	Samp.
	UNKNOWN	7,32	—	—	0,1967	—	—	—	Samp.
	UNKNOWN	7,34	—	—	0,0584	—	—	—	Samp.

- In the matching color codes

Above the results:



- In the horizontal bar

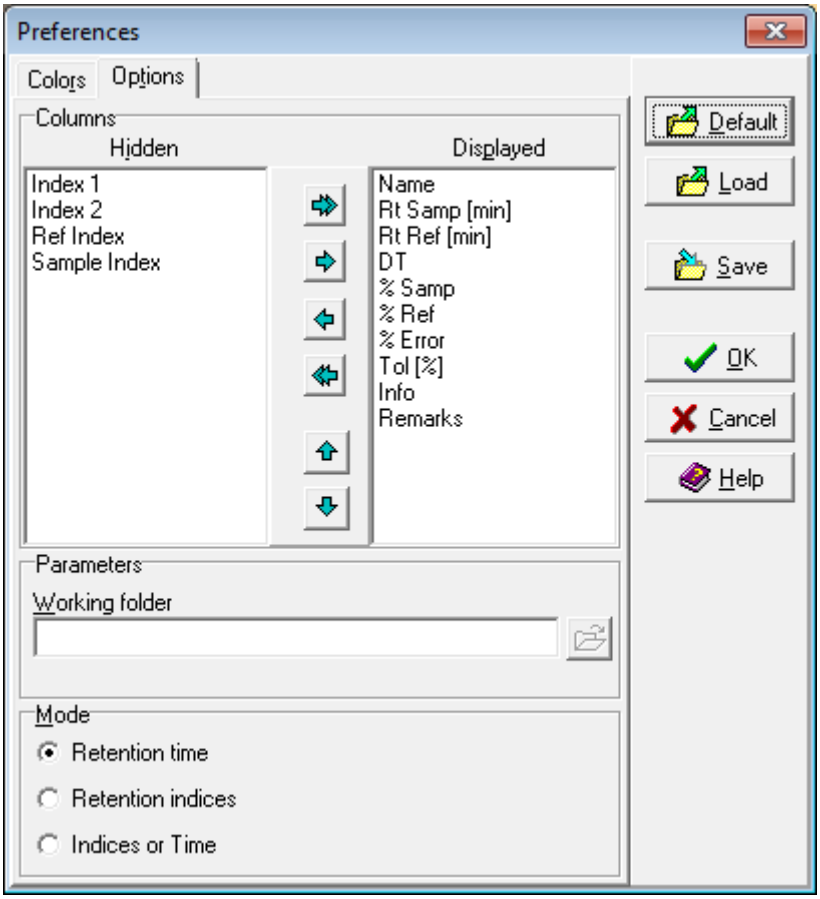
Options tab

The *Options* tab contains the following buttons:

Default : To return to default values.

Save : To save the modifications.

To customize the report (*Results* tab screen display, printing the comparison report and Excel export) select the desired columns and move them (with the *arrow* button) to the *Displayed* column. To remove selected columns, highlight and use the *arrow* button to move them to the *Hidden* column).



When all modifications are complete, click on the *Save*.

When all the modifications are complete in the module, validate by *OK*.

The modifications are applied to the following areas of the application.

- In the Results tab:

Name	DT	% Samp	% Ref	Info
UNKNOWN	------	0,0109	------	Samp.
UNKNOWN	------	------	6,3453	Ref.
UNKNOWN	-0,02	7,0622	8,8224	Id. HT , Tall peak
UNKNOWN	------	8,5487	------	Samp.
UNKNOWN	0,00	0,0289	0,0108	Id. HT
UNKNOWN	------	------	0,0042	Ref.
UNKNOWN	-0,02	0,0080	0,0049	Id. HT
UNKNOWN	-0,06	0,0066	0,0293	Id. HT
UNKNOWN	------	0,0315	------	Samp.
UNKNOWN	------	------	0,0017	Ref.
UNKNOWN	0,00	0,0090	0,0100	Id.
UNKNOWN	------	0,0274	------	Samp.
UNKNOWN	------	------	0,0314	Ref.
UNKNOWN	------	------	23,1232	Ref.
UNKNOWN	-0,11	25,0028	27,8692	Id. HT , Tall peak

- In the comparison report (Print preview):

Code	Name	DT	% Samp	% Ref	Info
	UNKNOWN	——	——	0,0093	Ref.
	UNKNOWN	——	——	0,0080	Ref.
	UNKNOWN	——	——	0,0239	Ref.
	UNKNOWN	——	——	0,0168	Ref.
	UNKNOWN	——	——	0,0096	Ref.
	UNKNOWN	——	——	0,0126	Ref.
	UNKNOWN	——	——	0,0130	Ref.
	UNKNOWN	——	——	0,0190	Ref.
	UNKNOWN	——	——	0,4682	Ref.
	UNKNOWN	0,00	0,4524	0,4694	Id. , Tall peak
	UNKNOWN	0,00	5,8732	5,7966	Id. , Tall peak
	UNKNOWN	——	0,0476	——	Samp.
	UNKNOWN	——	0,0098	——	Samp.
	UNKNOWN	——	8,9073	——	Samp.
	UNKNOWN	——	0,1967	——	Samp.

- In the Excel report

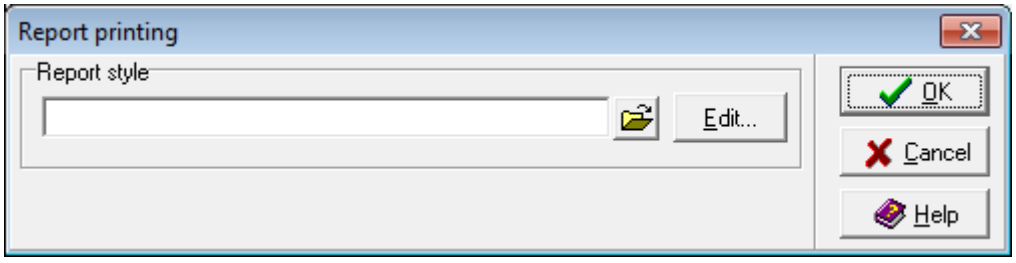
Name	DT	% Samp	% Ref	Info
UNKNOWI	------	0,0109	------	Samp.
UNKNOWI	------	------	6,3453	Ref.
UNKNOWI	-0,02	7,0622	8,8224	Id. HT , Tall peak
UNKNOWI	------	8,5487	------	Samp.
UNKNOWI	0	0,0289	0,0108	Id. HT
UNKNOWI	------	------	0,0042	Ref.
UNKNOWI	-0,02	0,008	0,0049	Id. HT

Comparison Report

Comparison Report Format

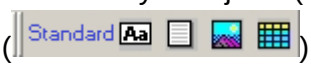
Creating and editing a style

Click on the *Print Preview* button ( ). The following screen is displayed:



Click on Edit. The CompassCDS Report Editor screen is displayed:

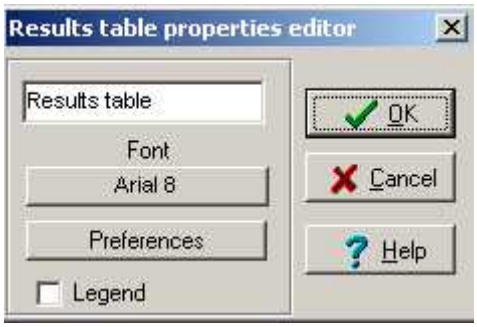
It contains CompassCDS ChromSync objects (

) and standards objects such as text, label, etc. (

), which allow you to build the report style.

Only CompassCDS ChromSync and text objects will be described above (for the other objects, refer to the *CompassCDS Report Editor* User Guide).

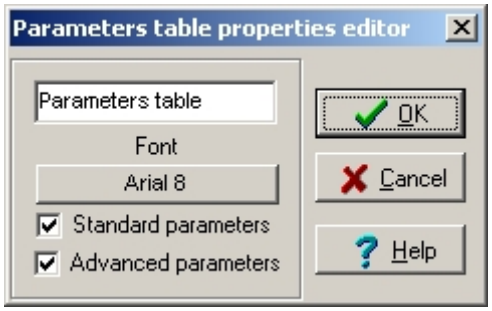
: By clicking on this icon, the user adds the result table to the report style. Right click on the object and select the *Properties* option. The following screen is displayed:



The user can choose to print (or not) the legend, to modify the results table font, colors, and the printed columns using the *Preferences* button.

The user can also change the results table title (if no title is specified, no title will be printed).

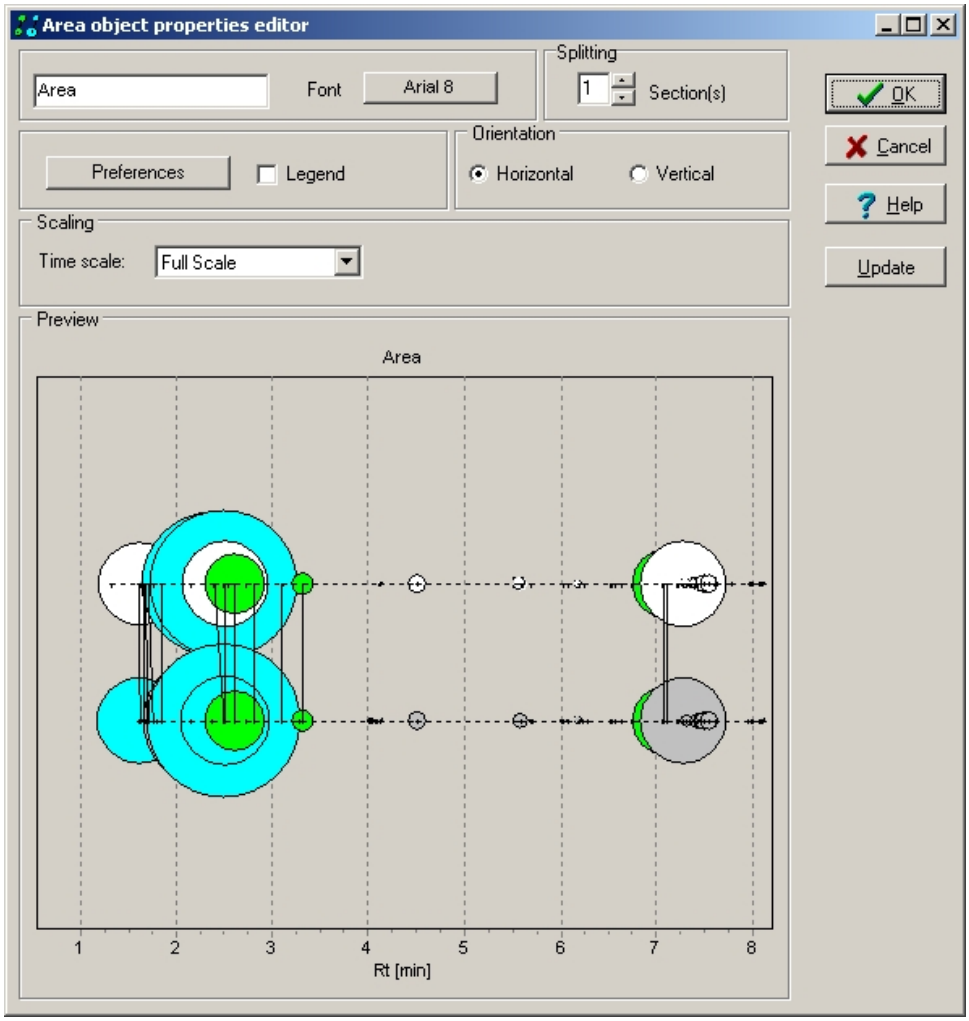
: By clicking on this icon, the user adds the comparison parameters table to the report style. Right click on the object and select the *Properties* option. The following screen is displayed:



The user can choose to print standard and/or advanced parameters and change the font.

The user can also change the parameters table title (if no title is specified, no title will be printed).

: By clicking on this icon, the user adds the results displayed in the *Areas* tab to the report style. Right click on the object and select the Properties option. The following screen is displayed:



The user can modify the color code (using the *Preferences* button).

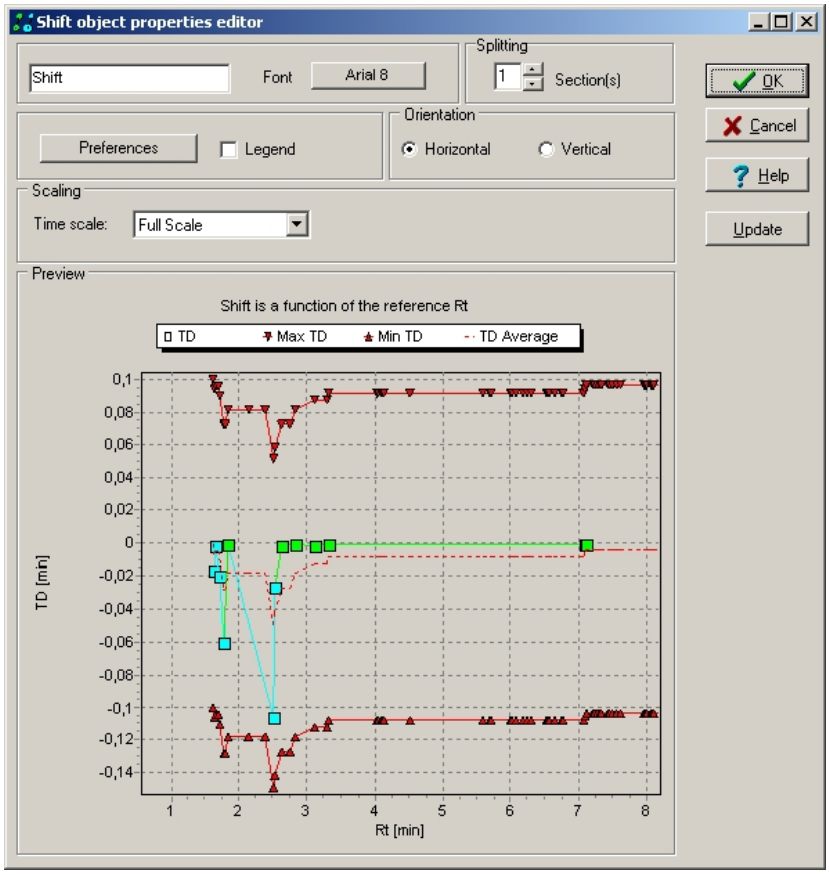
Printing the legend is optional, user can name the Areas object (if no title is specified, no title will be printed).

Area results can be printed in several parts corresponding to the number of sections specified in the *Splitting* field, either horizontally or vertically (*Orientation* parameter).

In the *Scaling* field, print either in *Full scale*, or select a specific time zone (*Custom* option), or a zone around a peak (according to its index or name (*Peaks#* or *named peak* options)).

In the preview, results can be viewed after an update.

: By clicking on this icon, the user adds the results corresponding to the *Shifts* tab to the report style. Right click on the object and select the *Properties* option. The following screen is displayed:



Modify the color code using the *Preferences* button.

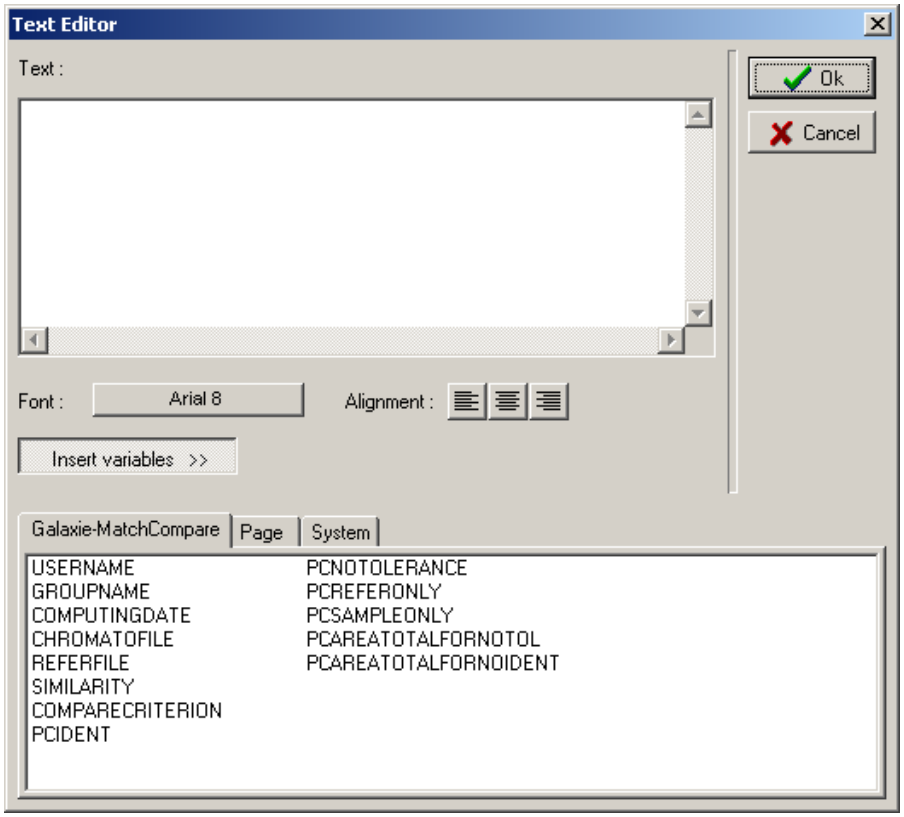
Printing the legend is optional. User can name the Time shift object (if no title is specified, no title will be printed).

Print shift results in several parts corresponding to the number of sections specified in the *Splitting* field, either horizontally or vertically (*Orientation* parameter).

In the *Scaling* field, print either in *Full scale*, or only a time zone (*Custom* option), or a zone around a peak (according to its index or name (*Peaks#* or *named peak* options)).

In the preview, results can be viewed after an update.

: By clicking on this icon, the user adds a text object to the report style. Right click on the object and select the *Properties* option. The following screen is displayed:



Print the text zone and variables (values have been automatically imported from CompassCDS ChromSync). Click on the *CompassCDS ChromSync* tab: several variables are displayed:

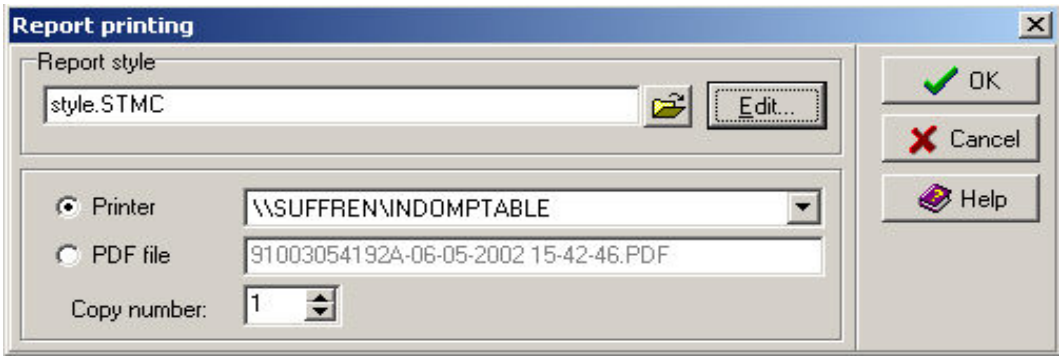
- USERNAME: name of the user (only available with CompassCDS application).
- GROUPNAME: name of the group (only available with CompassCDS application).
- COMPUTINGDATE: date of the processing.
- CHROMATOFILE: name of the sample chromatogram.
- REFERFILE: name of the reference file.
- SIMILARITY: similarity factor.
- COMPARECRITERION: this variable indicates if a success criterion has been selected (in the *Reference Definition* module).
- PCIDENT: percentage of matched peaks which verify the tolerance criteria.
- PCNOTOLERANCE: percentage of matched peaks which do not verify the tolerance criteria.
- PCREFERONLY: percentage of peaks which are only in the reference.
- PCSAMPLEONLY: percentage of peaks which are only in the sample.

- PCAREATOTALFORNOTOL: percentage of the total area corresponding to out of tolerance peaks.
- PCAREATOTALFORNOIDENT: percentage of the total area corresponding to non-identified peaks.

Double click to add one of these variables.

Format Selection – Printing

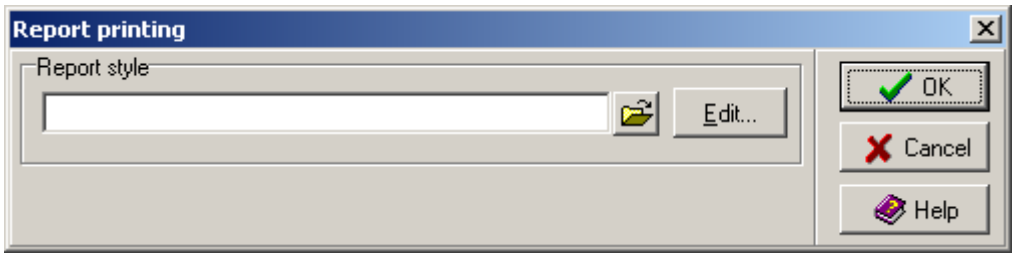
Click on the *Print* button ( ). The following screen is displayed:



Select the style in the corresponding file (button). Edit it by clicking on the *Edit* button.

The printer, PDF printing, and the copy number can be chosen. If you choose the *PDF file* option, a file is generated with the reference name, the date, and the printing time.

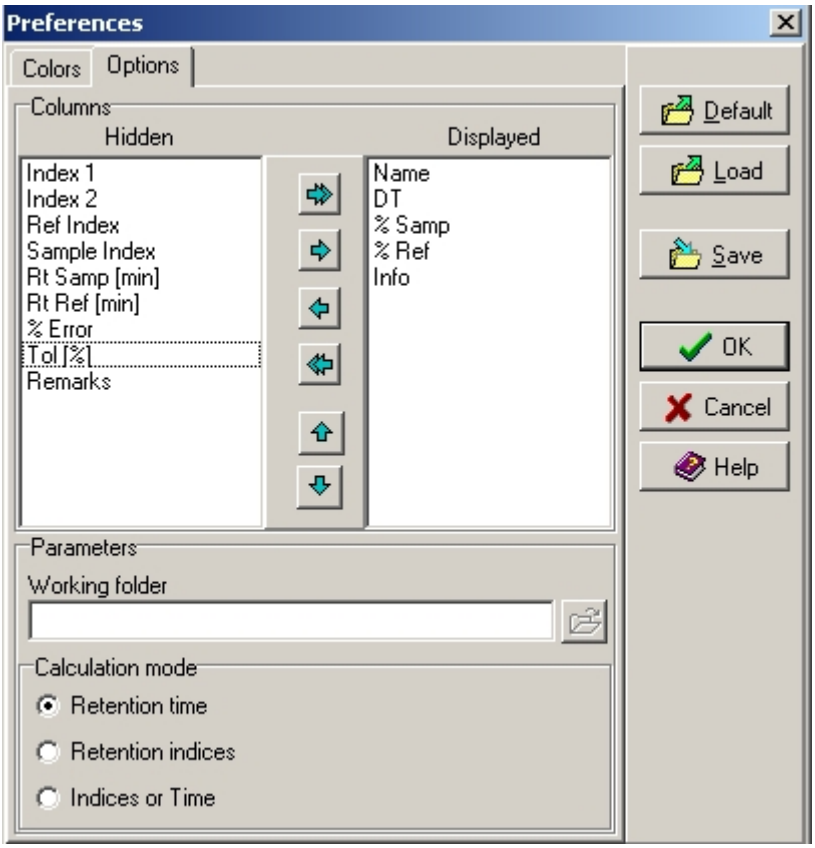
When you press the *Print Preview* button ( ), the following screen is displayed:



The report style can then be selected in the corresponding file (button), or edited with the *Edit* button.

Customizing the Report

To customize the report (*Preferences* window) select the appropriate columns and move them (with the arrow) to the *Displayed* column; to remove them, move them to the *Hidden* column.



- When the modifications are complete, click on the *Save* button.
- When all the modifications are complete in the module, validate by *OK*.

Excel Export

Customizing the report

If you changed the displayed columns in the Preferences window (Options tab), the modifications are updated in the Excel report.

By default, all the columns are displayed in the Excel report.

If the *Rt Samp, Rt Ref, % Error, Tol [%] and Remarks* columns are not selected, the following report is displayed:

	A	B	C	D	E
1					
2	Name	DT	% Samp	% Ref	Info
3					
4	UNKNOWN	------	0,0109	------	Samp.
5	UNKNOWN	------	------	6,3453	Ref.
6	UNKNOWN	-0,02	7,0622	8,8224	Id. HT , Tall peak
7	UNKNOWN	------	8,5487	------	Samp.
8	UNKNOWN	0	0,0289	0,0108	Id. HT
9	UNKNOWN	------	------	0,0042	Ref.
10	UNKNOWN	-0,02	0,008	0,0049	Id. HT
11	UNKNOWN	-0,06	0,0066	0,0293	Id. HT
12	UNKNOWN	------	0,0315	------	Samp.
13	UNKNOWN	------	------	0,0017	Ref.

Export

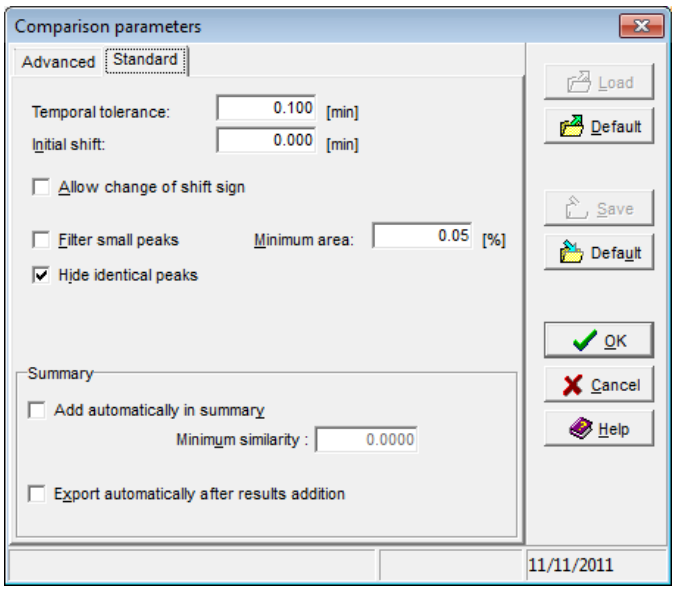
To export the result table, select the *FILE / EXPORT AS CSV* menu or click on the icon.

A .CSV file is created with the chromatogram name.

ChromSync summary

The comparison results between a reference and a sample file can be sent to a summary. This file is for saving merged results and it name is the reference file name with the file extension .merg. ChromSync generates a summary after the two modes of computation: retention times or retention indices.

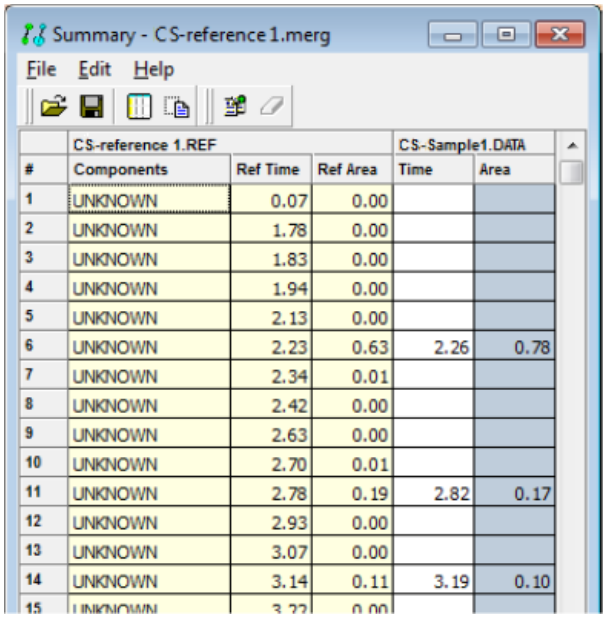
To create a new summary, select an option in the *Parameters* menu.



The addition to a summary is automatically done if the previous option is checked.

A minimum similarity value can be used for the summary addition. The comparison results whose similarity is less than the defined value won't be sent to the summary.

Each new summary created contains for each component, the component names, the theoretical indices 1 and 2 (in retention indices mode), the reference times (or retention indices), the reference area.



	CS-reference 1.REF			CS-Sample1.DATA	
#	Components	Ref Time	Ref Area	Time	Area
1	UNKNOWN	0.07	0.00		
2	UNKNOWN	1.78	0.00		
3	UNKNOWN	1.83	0.00		
4	UNKNOWN	1.94	0.00		
5	UNKNOWN	2.13	0.00		
6	UNKNOWN	2.23	0.63	2.26	0.78
7	UNKNOWN	2.34	0.01		
8	UNKNOWN	2.42	0.00		
9	UNKNOWN	2.63	0.00		
10	UNKNOWN	2.70	0.01		
11	UNKNOWN	2.78	0.19	2.82	0.17
12	UNKNOWN	2.93	0.00		
13	UNKNOWN	3.07	0.00		
14	UNKNOWN	3.14	0.11	3.19	0.10
15	UNKNOWN	3.22	0.00		

ChromSync searches for all the components added to the summary a component with the same reference time (or retention index):

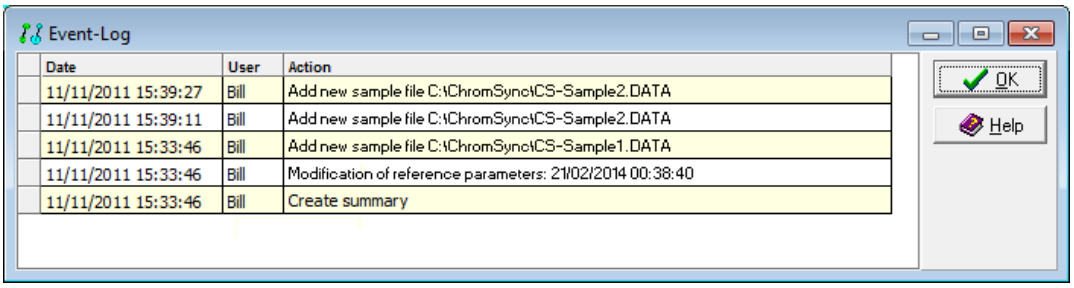
- If a reference component is found, the software adds to this reference the sample component time (or retention index) and the sample component area.
- If a reference component is not found, the software adds a new reference component. It fills the old comparison results already added to in the summary with null values and adds current comparison results.
- If the new comparison has no reference component, it corresponds to a “sample only”. The software creates a new reference component with the same time as the sample component. This new reference component is identified as a “virtual” reference component.

The user can delete one or more comparison results or add the current comparison.

The user can add a summary object to a ChromSync report style to print the array which merges the comparison results.

The user can export a selected summary file. A parameter in the Preferences menu allows the user to generate an export automatically after comparison. Export of ChromSync summary creates a .csv file with semi-colon for array column separator.

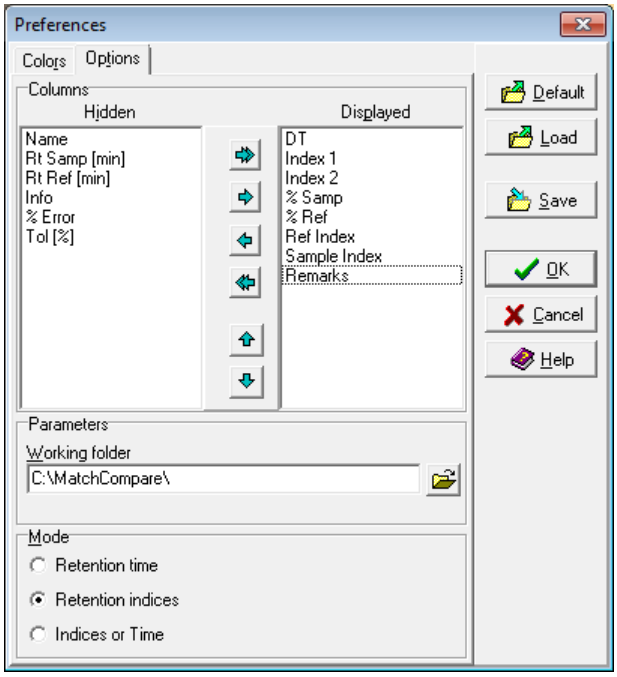
An event-log is saved within the summary file and is updated after each action (add result, print, export, editing, etc.). This event-log lists the action done, the date, the user connected in Windows.



Specific Case: Retention Indices

Reference and sample can be compared with retention indices instead of retention time.

Select the *EDIT / PREFERENCES* menu and click on the *Options* tab. The following screen is displayed:



In the *Calculation mode* parameter group select either *Retention time* or *Retention indices*, according to the desired comparison.

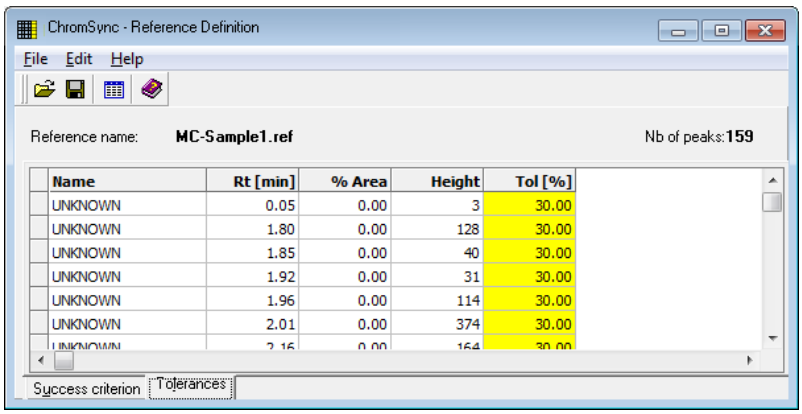
If the *Indices or time* option is selected, chose the calculation mode. (This option cannot be used when using ChromSync plug-in. If this option is checked, the Index mode is used if indices are defined in the sample, otherwise time mode is used).

NOTE: The *Indices or time* option can be used only in manual (direct call) mode. If you are using the CompassCDS ChromSync plug-in in post-run, this option must not be selected. In this case, the Index mode is used if indices are defined in the sample. Otherwise, time mode is used.

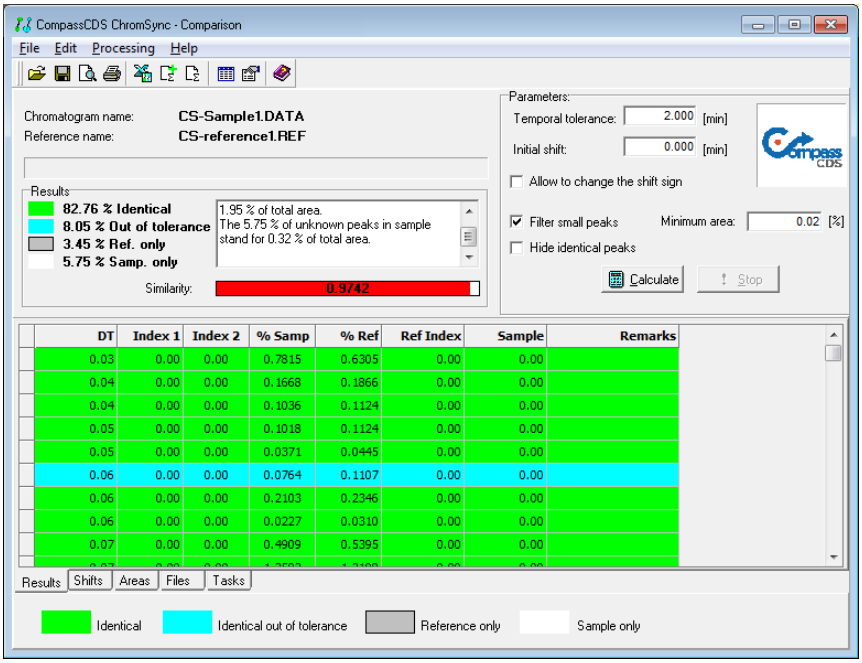
If you answer *Yes* to the confirmation message (Do you want to compare the indices?), the comparison will be generated with retention indices.

If you answer *No*, it will be generated with retention times.

The comparison algorithm is the same as the retention time algorithm. A new column is displayed (*index* column) in the *Reference Definition* window.


ChromSync - Reference Definition
File Edit Help
Reference name: MC-Sample1.ref
Nb of peaks:159
Name | Rt [min] | % Area | Height | Tol [%]
UNKNOWN | 0.05 | 0.00 | 3 | 30.00
UNKNOWN | 1.80 | 0.00 | 128 | 30.00
UNKNOWN | 1.85 | 0.00 | 40 | 30.00
UNKNOWN | 1.92 | 0.00 | 31 | 30.00
UNKNOWN | 1.96 | 0.00 | 114 | 30.00
UNKNOWN | 2.01 | 0.00 | 374 | 30.00
Success criterion
Tolerances

The results and parameters form setup to retention indices:


CompassCDS ChromSync - Comparison
File Edit Processing Help
Chromatogram name: CS-Sample1.DATA
Reference name: CS-reference1.REF
Parameters:
Temporal tolerance: 2.000 [min]
Initial shift: 0.000 [min]
Allow to change the shift sign
Results
82.76 % Identical
8.05 % Out of tolerance
3.45 % Ref. only
5.75 % Samp. only
1.95 % of total area.
The 5.75 % of unknown peaks in sample stand for 0.32 % of total area.
Similarity: 0.9742
Filter small peaks
Minimum area: 0.02 [%]
Hide identical peaks
Calculate
Stop
DT | Index 1 | Index 2 | % Samp | % Ref | Ref Index | Sample | Remarks
Results Shifts Areas Files Tasks
Identical
Identical out of tolerance
Reference only
Sample only

Parameters fit retention indices (for example, the temporal tolerance is replaced by a tolerance on indice, etc.).

In the comparison module, reference and sample indices appear in the Results tab. The DToll column (as DT) indicates the difference between Reference and Sample indices.

Tips and Examples

This section describes tips on working with large directories in CompassCDS ChromSync and a series of examples: sensitive area within chromatograms and use of comparison parameter values different from the default one.

Working with Large Directories

Be careful: this section may be useful when working with a standalone ChromSync version only.

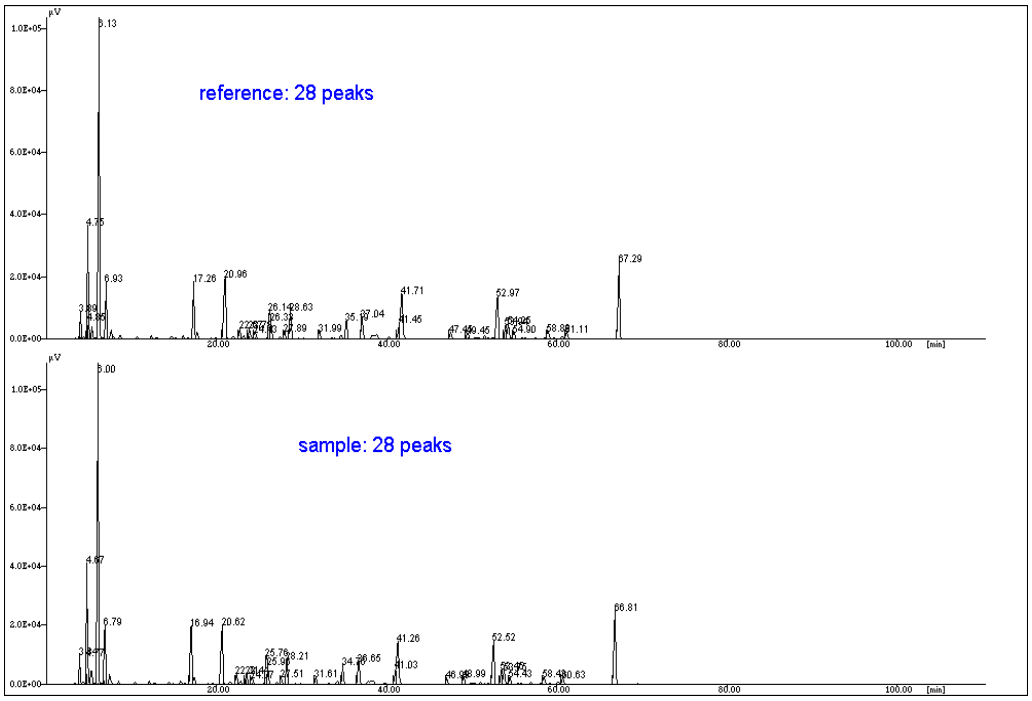
When your directory contains a great number of files (around 1000 chromatograms for example), opening this directory could take a long time. You can reduce this time by using the following procedure:

- Open ChromSync and the Windows Explorer (or another one) in Windows office.
- Select the files in the explorer by using the CTRL touch: the selected files are displayed in blue.
- Click and drag the selected files to ChromSync:

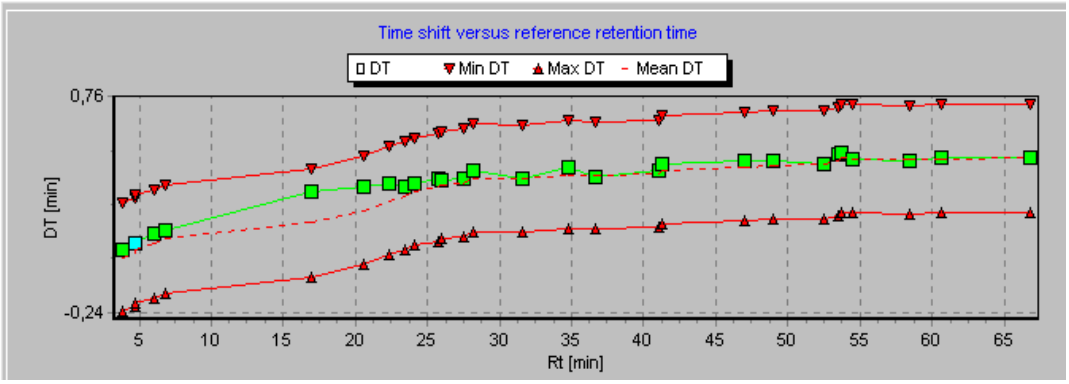
If only one file has been selected, you access the Reference module. Then you can define the reference file.

When several files have been selected in the explorer, ChromSync compares the reference chromatogram with the sample chromatogram which has first been selected. The corresponding sequence list is also built and displayed in the *Tasks* tab.

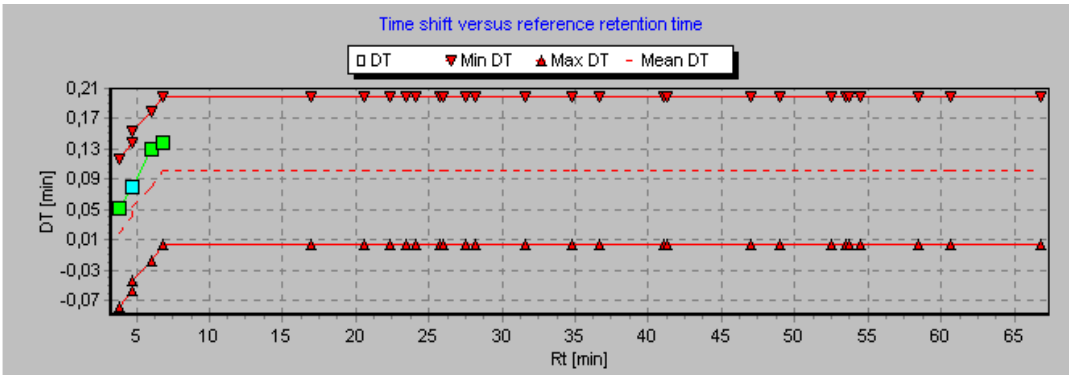
Influence of Temporal Tolerance



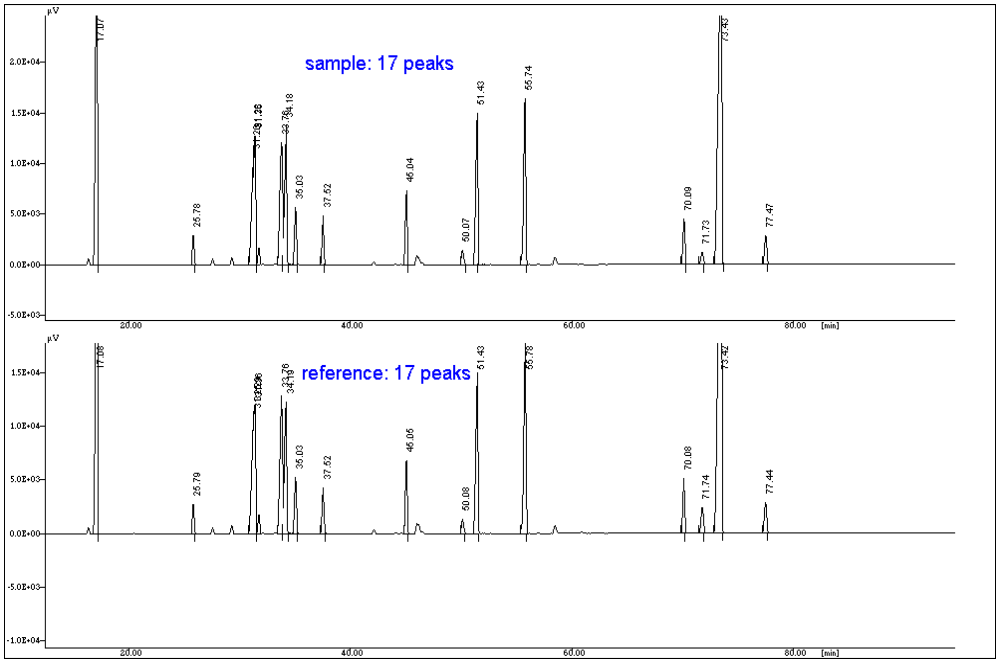
When temporal tolerance equals 0.25 min, the comparison between the two chromatograms gives very good results (similarity equals 1). The diagram corresponding to the time shift versus the reference retention time shows a difference between the average shift and the time shift (DT): in fact, from 7 min to 22 min, the time shift tends to get closer to the maximum shift.



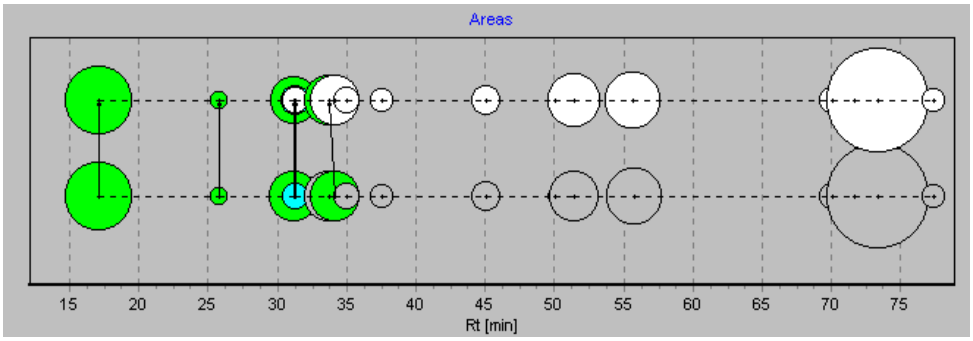
When temporal tolerance is too low (0.1 min for example), the shift becomes superior to the temporal tolerance which can explain the bad results (a few peaks are matched).



Influence of the Shift Sign



Theoretically, all peaks are matched. If the comparison is performed with the default parameters, similarity is very bad and unknown peaks represent 43.6% of total area.



In fact, the sign of shift changes as you can see in the results peak by peak:

Name	Tr Samp (min)	Tr Ref (min)	DT	% Samp	% Ref
Unknown	17.07	17.08	-0.01	13.5832	13.844
Unknown	31.20	31.25	-0.05	6.4741	7.0809
Unknown	33.76	33.76	0.00	7.5297	7.1720
Unknown	73.43	73.42	0.01	31.1367	31.7195
Unknown	77.47	77.44	0.03	1.5664	1.5232

If the sign shift is allowed to change, all peaks are correctly matched.

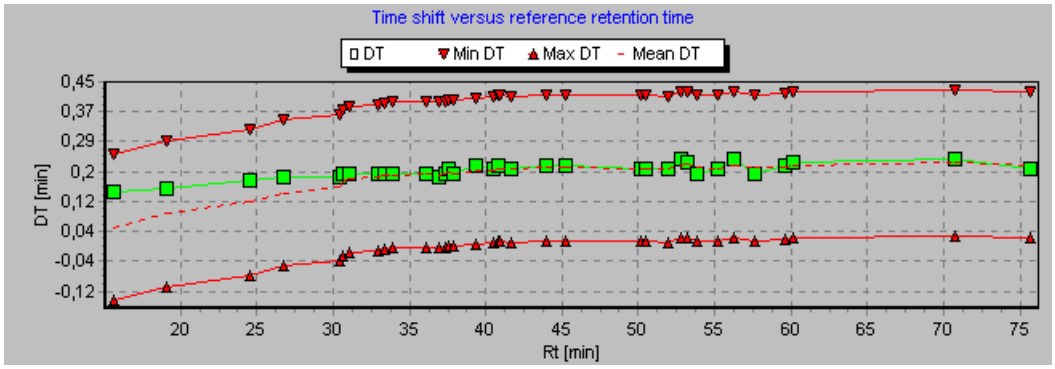
Influence of the Initial Shift

Two chromatograms (reference and sample) presenting the same number of peaks are considered.

The first comparison was performed with the following parameters:

- Temporal tolerance: 0.2 min
- Initial shift: 0.00 min

The corresponding time shift curve appears below:

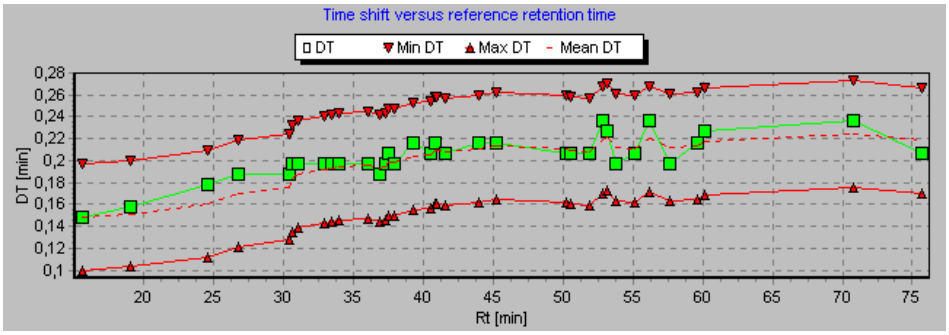


Of course, matches are correct: the 2.78% of unknown peaks represent 0.42% of total area. This corresponds to one supplementary peak in the sample chromatogram. Similarity equals 0.9810. But if we consider the time shift versus the reference retention time, we can see an initial shift on the diagram.

So, another comparison was performed with the following parameters:

- Temporal tolerance: 0.05 min
- Initial shift: 0.15 min

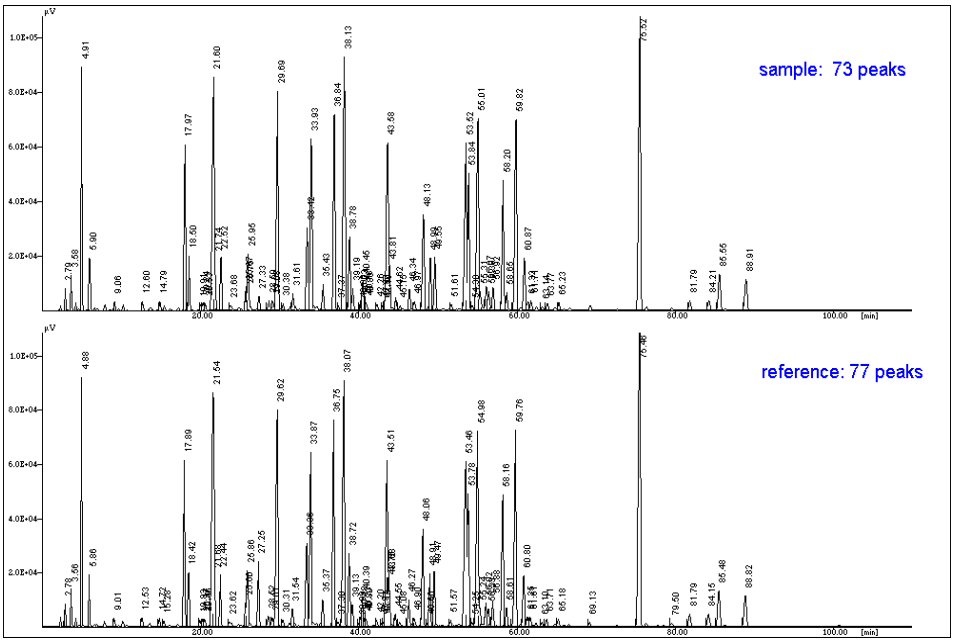
These new parameters lead to the same results as before but if the initial shift is considered, temporal tolerance can be reduced.



NOTE: When an initial shift exists and when the user knows it, it will be necessary to specify it in the standard parameters: as a consequence, temporal tolerance could be reduced and erroneous matches will be avoided.

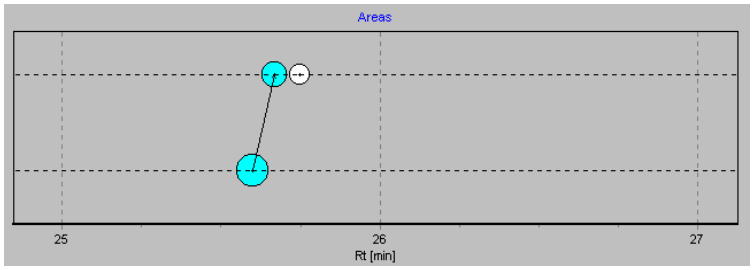
Sensitive Areas within Chromatograms

Example #1



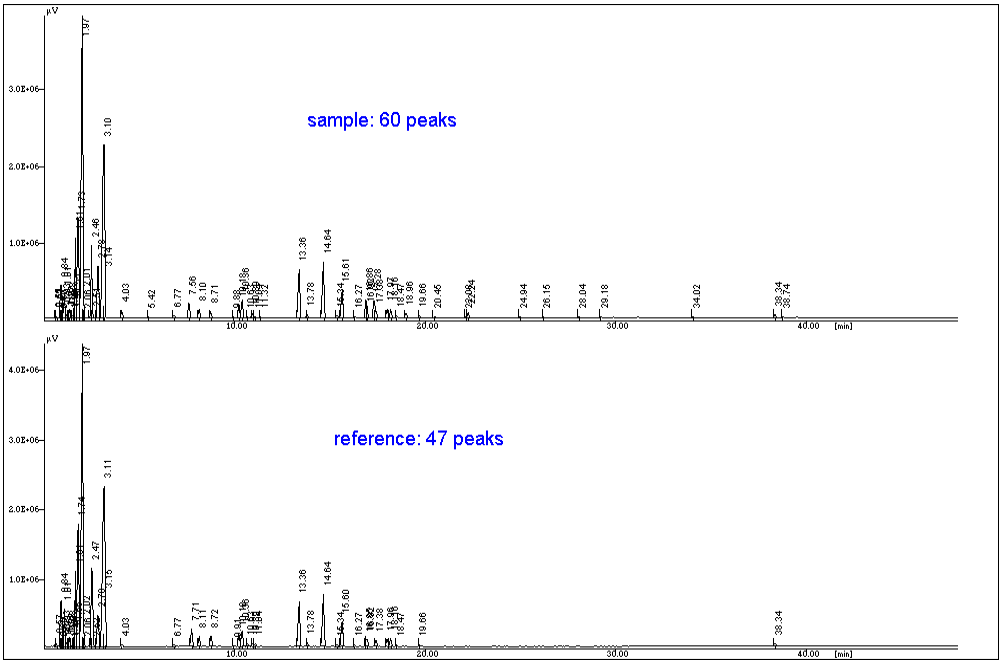
CompassCDS ChromSync correctly identifies the four peaks which are present only in the reference chromatogram. Moreover, the comparison underlined one sensitive area: the reference peak at 25.60 min appears as two neighboring peaks in the sample chromatogram as you can see in the following table:

Name	Tr Samp (min)	Tr Ref (min)	DT	% Samp	% Ref	% Error
Unknown	25.67	25.60	0.07	0.3624	0.5917	-38%
Unknown	25.75			0.2175		

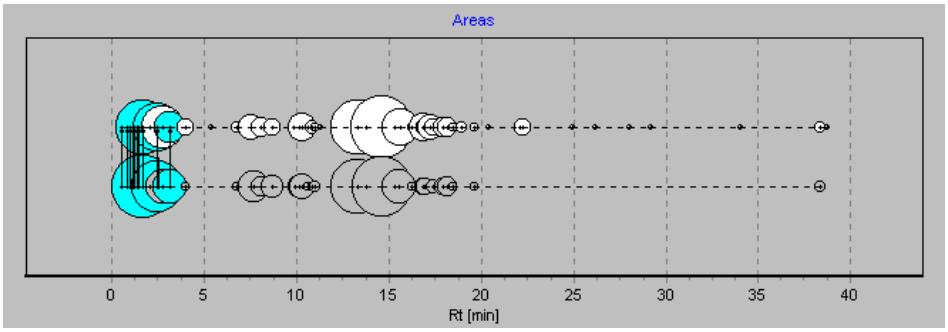


Finally, CompassCDS ChromSync suggests a match whereas the other peak (Tr = 25.75 min) is considered as isolated.

Example #2

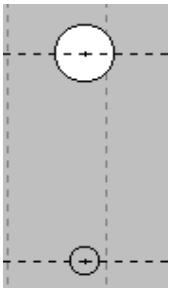


The comparison between the reference and the sample by using the parameters default values gives the following results (identical peaks are hidden):



A lot of peaks are not coupled whereas they seem to be identical. Moreover, similarity is very bad.

Explanation: on the one hand, the sign of some shifts changes; on the other hand, one compound presents an error percentage superior to the default value which is defined in the advanced parameters (200%).

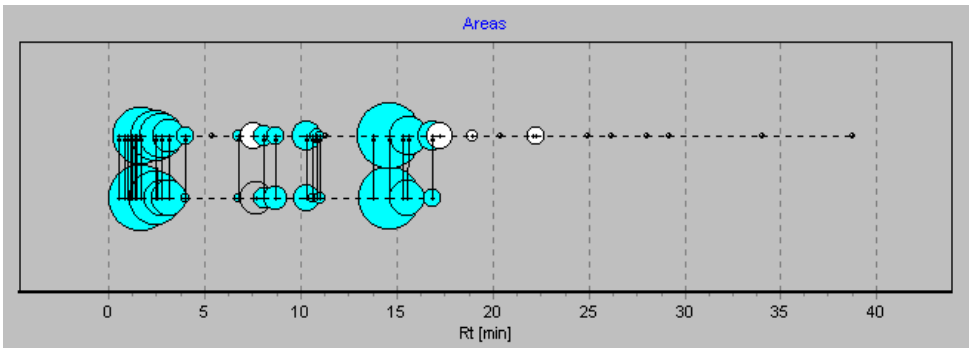


This zoom shows the difference between the reference peak area and the sample peak area.

The comparison becomes correct by using the following parameters:

- Maximum error: 300%
- Number of sample peaks: 10 (if the default value is maintained, some peaks are not matched).

Similarity equals 0.9079.



CompassCDS
ChromSync
Release Notes

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501545
Revision A

What’s New in ChromSync Version 2.0

Compatibility

ChromSync can be installed on CompassCDS 2.x , 3.x, and 4.x, and Galaxie 1.9 and 1.10

USB dongle

The USB dongle protection has been removed

What’s New in ChromSync Version 1.5

Compatibility

ChromSync can be installed on Galaxie 1.9 and Galaxie 1.10 with ChromSync setup version 97 or above

USB dongle

The parallel dongle has been replaced by a USB dongle

Demo version

A ChromSync Demo version is now available

What’s New in ChromSync Version 1.4

Summary

A summary has been added, allowing the user to list the comparison made between one reference and one or several samples. Comparison results are displayed and can be exported.

Relative Mode Calculation

Provided the user has not validated the relative mode in the preference screen, the main screen is not updated. However, the calculations and the report consider this calculation mode.

Scion 400 Series GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501497
Revision C

Contents

Introduction 3
General 3
Installation and Configuration 3
Installing the Driver Software 3
Configuring the GC Communications 3
Ethernet Communications 3
Configuring the Driver 3
Configuring the 400 Series GC 3
Configuring the Synopsis 5
Building a Method 8
Creating a New Method 8
Control Method Section for the 400 Series GC 10
AutoSampler Control 11
Injectors Control 23
Column Oven Control 28
Column Pneumatics Control 30
Detectors Control 35
Output Ports Control 43
Valves Control 44
Auxiliary EFCs 45
Starting and Viewing an Acquisition 48
Quick Start and Sequence 48
Quick Start (Single Acquisition) 48
Sequence 49
Running Acquisition Status 49
Viewing a Running Acquisition 49

Introduction

General

This document describes the configuration of the Scion/Bruker/Varian 400 Series GC control driver (models; 450 GC, 451 GC, 436 GC and 456 GC). It also explains how to build a control method for this driver, how to start and view a running acquisition, and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS Installation Guide.

Configuring the GC Communications

Ethernet Communications

The 400 Series GC uses Ethernet® as the method of communications for instrument control.

The 400 Series GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server can be used to assign IP addresses but the recommended procedure is to assign a static IP address in the GC.

To know how to configure the BOOTP server, refer to the CompassCDS installation Guide.

NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the 400 Series GC

Click on the button corresponding to the 400 Series GC driver and the GC configuration screen appears.

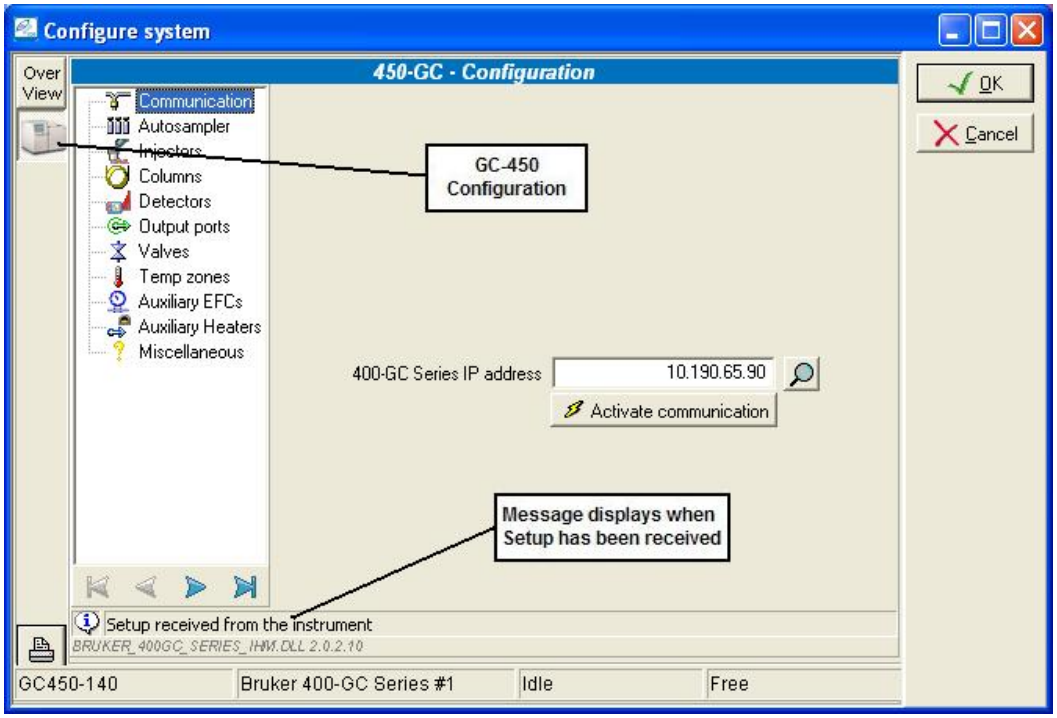
The toolbar allows you to easily scroll through the configuration windows:

to select the first configuration window.

to select the previous configuration window.

to select the next configuration window.

to select the final configuration window.



Select the **Communication** sub-section and enter the IP address of the 400 Series GC (configured in the BOOTP server) or click on the button to find the instrument previously configured with the BOOTP server program and select it.

Press the

button to automatically get the configuration from the instrument.

As soon as the configuration of the instrument is received the name of the instrument type 450/451/436/456-GC is displayed in the title of each driver window (configuration, method and status).

Select the following sub-sections to see the corresponding module configurations (the screens displayed are read-only screens):

Autosampler: displays the autosampler type if installed, the autosampler position, the number of injection ports, the syringe volume or type.

Injectors: displays, for each injector identified by its location (Front, Middle, Rear), the injector type, the installed temperature zone, the associated injector EFC type if installed, the outlet pressure, the pressure display units, the splitless vent flow, the gas saver flow, the gas saver timeout, the column septum purge head pressure and the septum purge flow rate.

Columns: displays whether the column is installed or not (the location -Front, Middle, or Rear- refers to the sample introduction device to which the column is connected), the corresponding temperature zone and the column parameters, which include the carrier gas, the capillary column length and ID (Inside Diameter). If a packed column is used, then 0 is set for length and ID. The carrier gas and column dimension information is used for EFC calculations. Also the pressure units are displayed. The pressure units can be changed to psi, kPa or bar for each position. This setting

converts the pressure values of the injector EFCs in the status and method screen of CompassCDS to the preferred unit.

Detectors: displays the detector type for each location (Front, Middle, Rear), the corresponding temperature zone, the corresponding EFC type if installed, channel 1, 2, 3 gas types according to the installed EFC, and the supported detector frequencies.

Valves: displays the name of the installed valves. Seven internal events and eight external events (using an option board) are available on the 400 Series GC. When a name has been chosen in the instrument setup, this also defines the default states of the valve. These states will be visible when the valve is being programmed in the valve control section of the 400 Series GC method.

Temp zones: displays the six available heated zones on the 400 Series GC and the column oven heated zone. All zones have temperature programming capability and three (Coolable zones 1 - 3) have cryogenic cooling capability. Typically, Coolable zones 1 - 3 are assigned to injectors and Heat-only zones 4 - 6 to detectors.

Auxiliary EFCs: displays added auxiliary EFCs. EFCs can be placed in front, middle and rear position.

Auxiliary Heaters: displays added auxiliary heaters.

Miscellaneous: displays all kind off instrument version information.

NOTE: If you want to modify the GC configuration, you need to use the Setup button directly on the instrument front panel. The 400 Series GC is configured at the factory, and you need to enter Setup only when hardware is being installed such as a column or a field upgrade is done or an option is removed. Refer to the instrument manual for more details.

Configuring the Synopsis

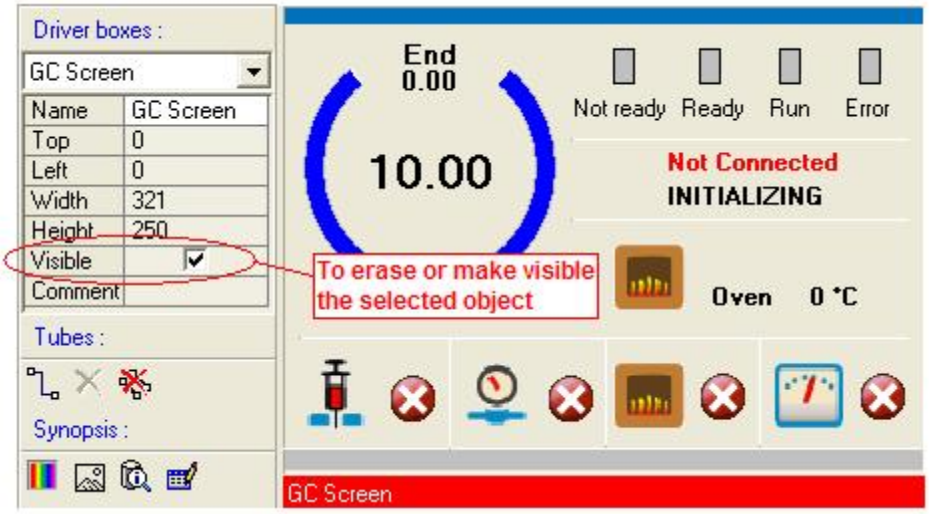
In the *Overview* part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

1. To save the configuration of these devices, click on the *OK* button.
2. Right click on the system name in the bottom part of the ***CompassCDS Configuration Manager*** screen. A pop-up menu appears: click on *Stop.* Then right click on the system name again, and click on *Start*.

1. Go back to the System Configuration screen (***Properties*** wizard). A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, then connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

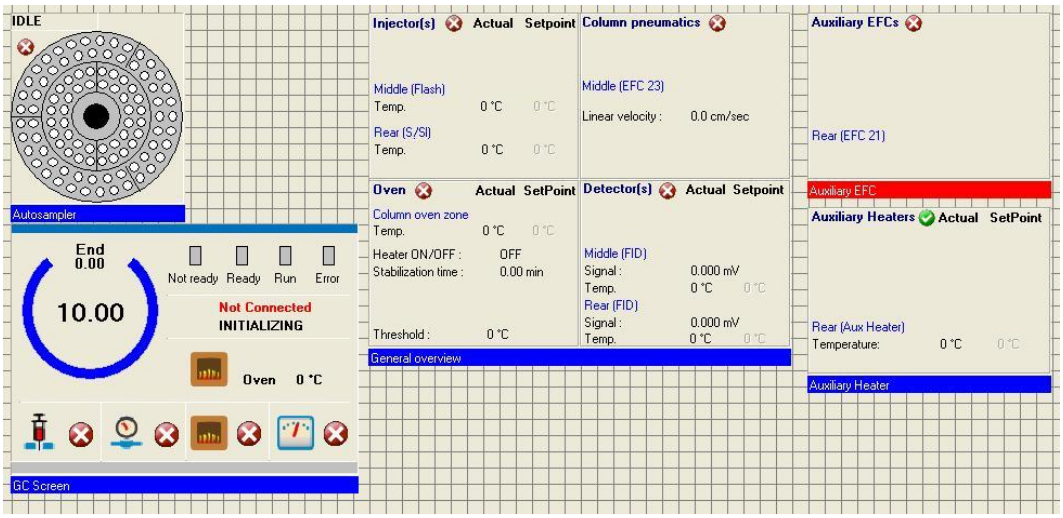
2. Click on the to delete a selected tube, click on the button to delete all the tubes. Click on to define a background color, or on to make the background transparent. Click on the icon to change the grid color.

3. You can choose which screen will be visible or not if you consider that some screen should not be displayed on the Overview: just check or uncheck the Visible box



1. Once the synopsis configuration is complete, it will be displayed in CompassCDS in the *Systems* tab. In this tab, the *Overview* part will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.) depending on the installed devices.

2. For example, the following pictures represent the synopsis of the 400 Series GC:



CompassCDS Configuration Manager screen

CompassCDS Chromatography Data System screen

NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Click on the button to print the current configuration.

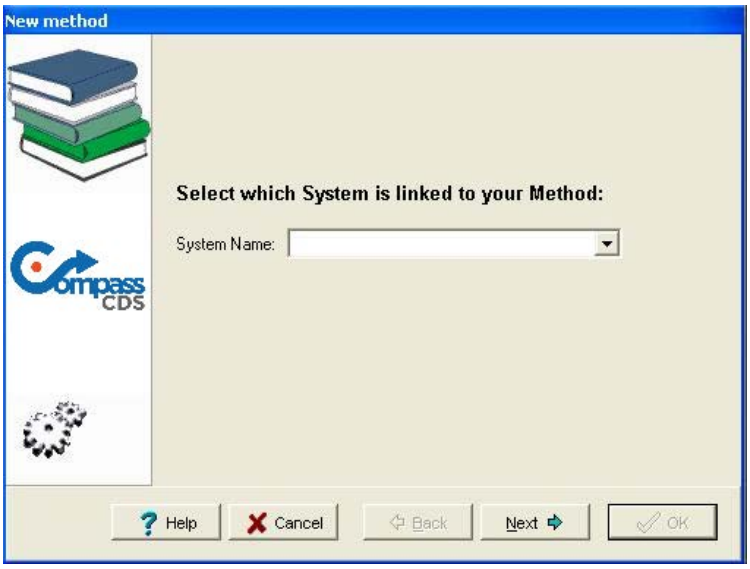
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument section prior to starting an acquisition.

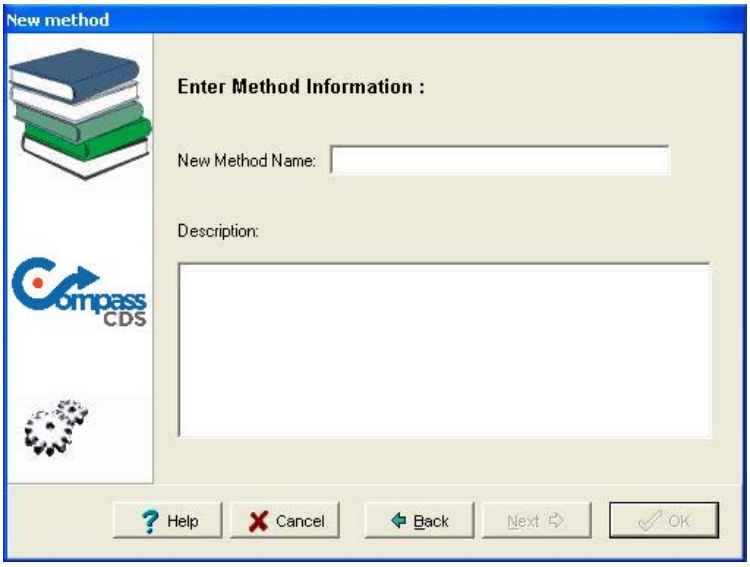
1. To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS main menu.

   A wizard guide will appear and provide assistance during the first steps of method creation:



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

3. Once this field is completed, click on the *Next* button to move to the second step of the method creation:



4. Enter the *New Method Name* in the first field. In the *Description* field, enter information concerning the method (optional).

5. Once these two fields have been completed, click on the *OK* button. The new method is created and is opened with default parameters in CompassCDS. The next step is the definition of each of the method sections.

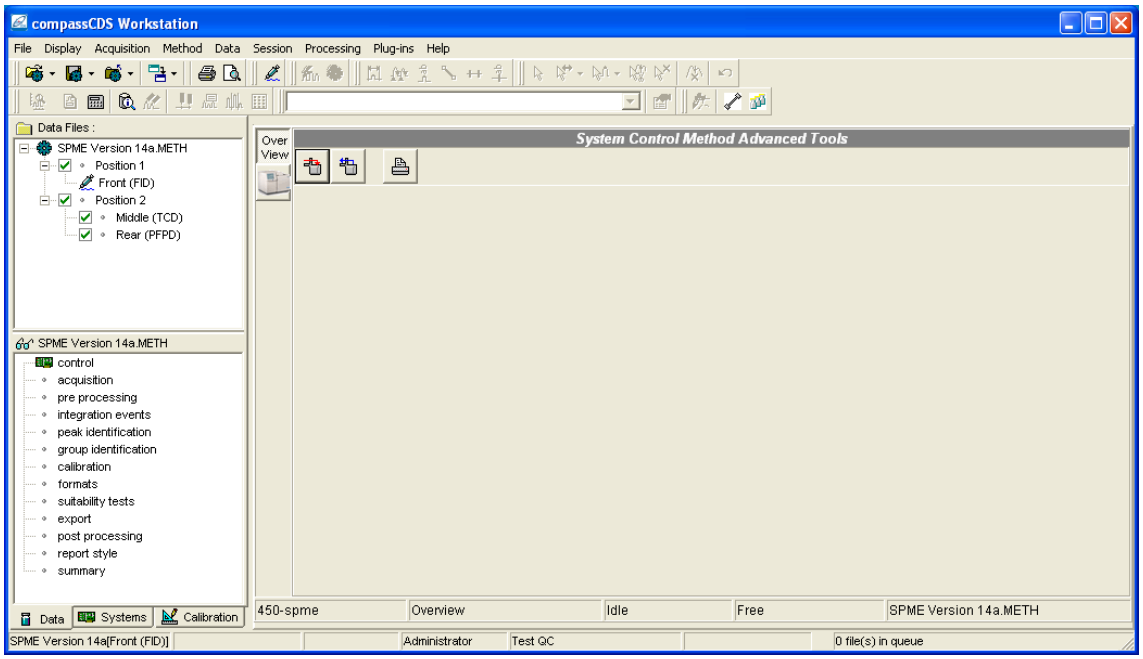
The instrument *control* section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the 400 Series GC is detailed. Other parameters such as *Injection Volume*, *Vial* and *Rack* number may be necessary and are defined in the *acquisition* section.

NOTE: For more details about the programming of each method section, refer to the CompassCDS User Guide.

Control Method Section for the 400 Series GC

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



Press the Over View button to display the ***System Control Method Advanced Tools*** window:

To send the current method to the instrument.

To get the active method from the instrument.

To print the current method.

Click on the button to display the 400 Series GC control method section. It contains eight sub-sections: *Autosampler*, *Injectors*, *Column oven*, *Column pneumatics*, *Detectors*, *Output ports*, *Valves*, and *Miscellaneous*. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

The toolbar allows you to easily scroll through the control method windows:

to select the first window of the control method.

to move back to the previous window of the control method.

to move forward to the next window of the control method.

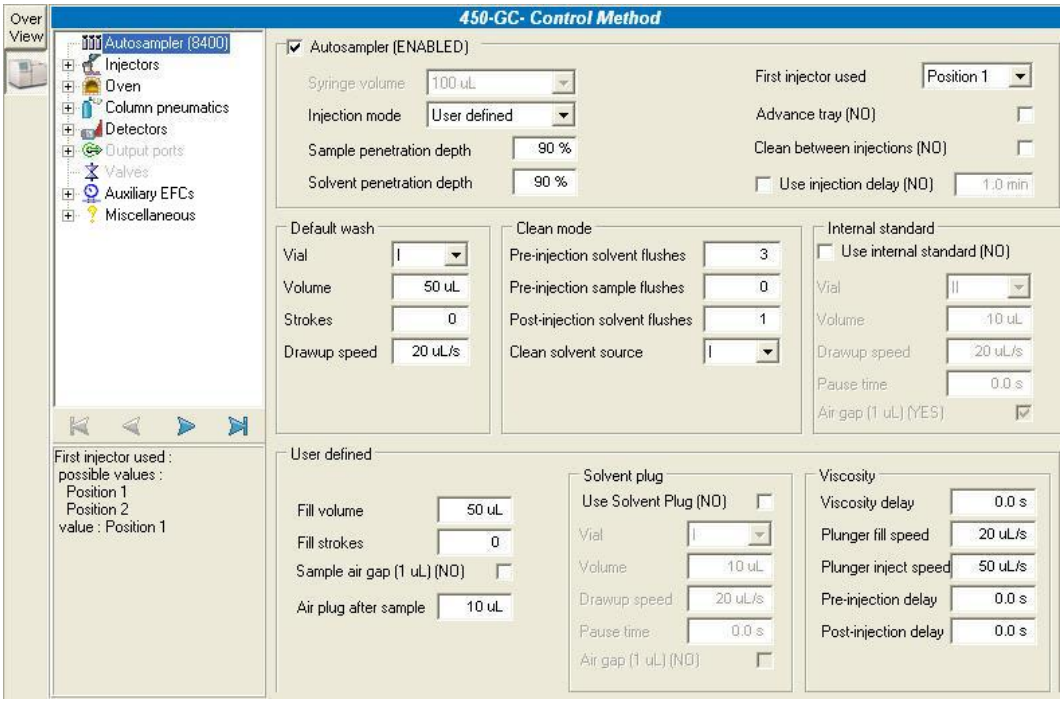
to select the final window of the control method.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

AutoSampler Control

The AutoSampler window contains sampling parameters for the 8400/8410 AutoSampler when attached to the 400 Series GC:

Liquid Mode



Autosampler parameter group

In this parameter group, the sampling syringe size (in read only mode, the value displayed corresponds to the one defined in the instrument), the penetration depth for sample and solvent wash vials, the injection mode, and injector position.

Dual and Duplicate injections using the 400 Series GC with two injectors, the 8400/8410 AutoSampler and CompassCDS.

The CompassCDS software will support the 8400 Dual and Duplicate modes of operation on the 400 Series GC appropriately equipped with two injectors. Dual injection mode allows an operator to inject samples from two adjacent vials into both a front and back injector that lies on the arc of the 8400/8410 tower. Duplicate mode injections allow an operator to inject from the same vial into both injectors as described above. To use these features, you must perform certain steps for both the 400 Series GC 8400 setup and for CompassCDS.

Configuring the 400 Series GC 8400/8410

CompassCDS will read the configuration from the GC and will use it to configure itself to either use one injector only or to allow dual and duplicate injections as well as single injections. To configure the 400 Series GC for dual and duplicate injections:

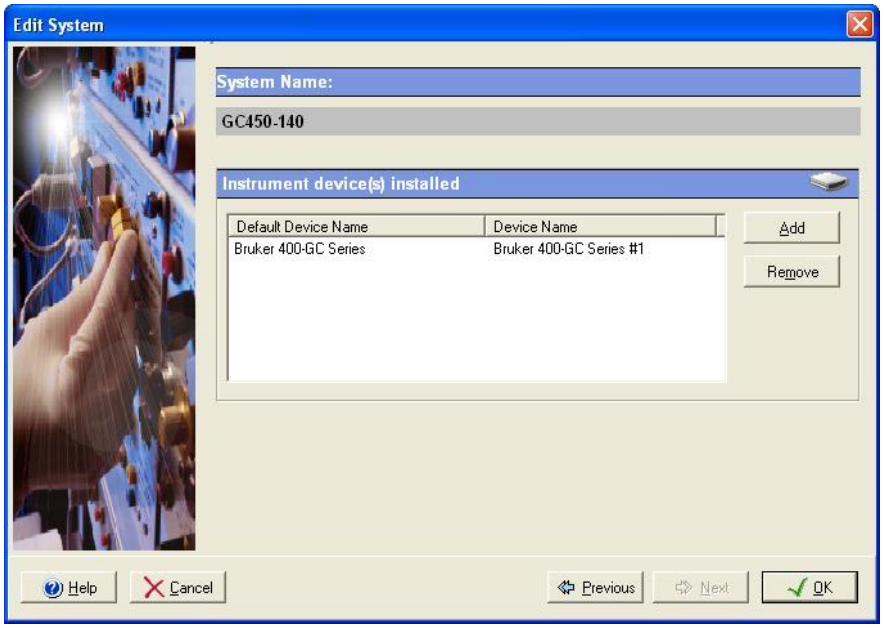
- Press the Setup key on the 400 Series GC keyboard
- Select Edit Instrument Setup
- Select Edit Sample Delivery Parameters
- Set the Sampler Injection Position to Both
- Save and Exit Setup; the 400 Series GC will reboot.

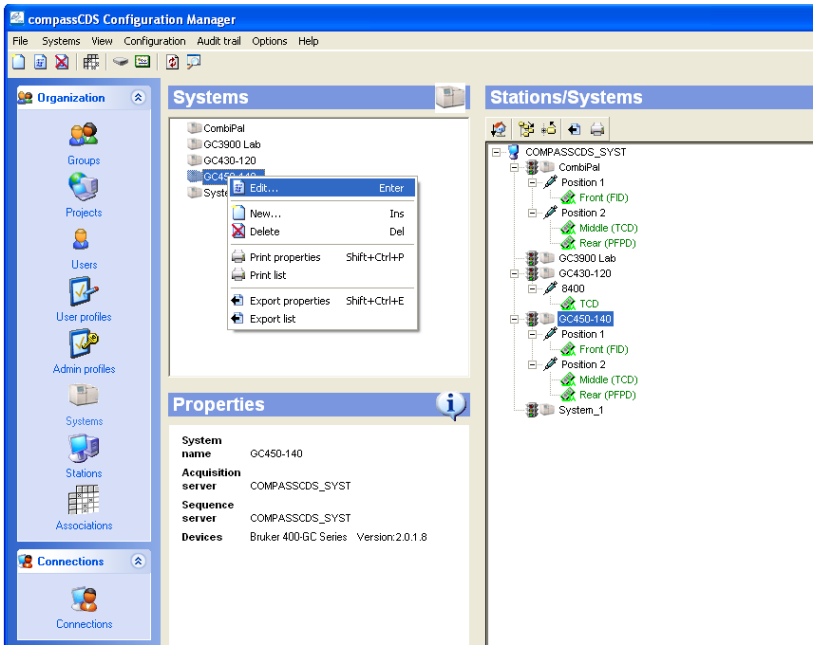
It is assumed that you have calibrated the 8400/8410 for both the front and back injector positions that you will be using. If you have not done this, you should make certain the calibration is done before you start using your system.

Configuring CompassCDS

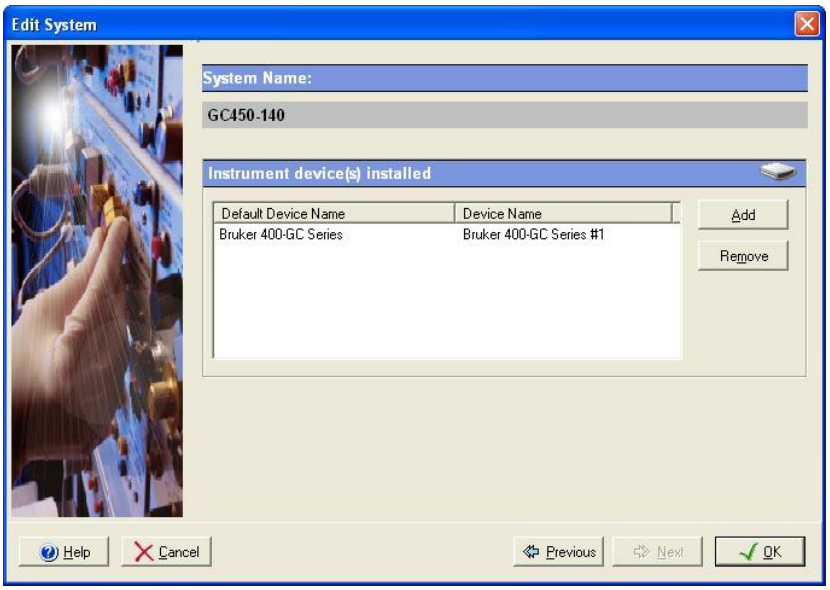
To configure CompassCDS you will first have to add the system you are using if you have not already done so.

Follow the instructions in the CompassCDS Manuals for creating a new system. If you already have a system right-click on the system and choose edit; follow the instructions below.

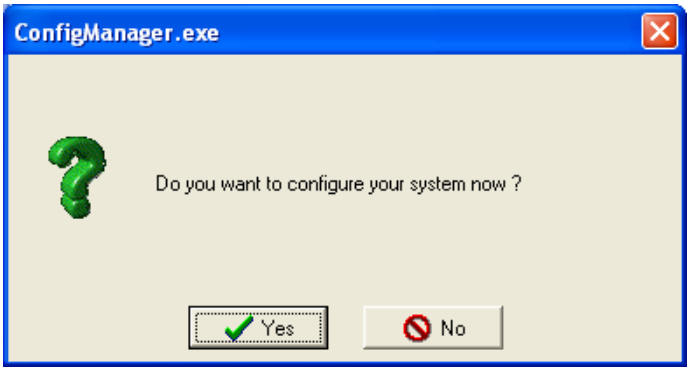




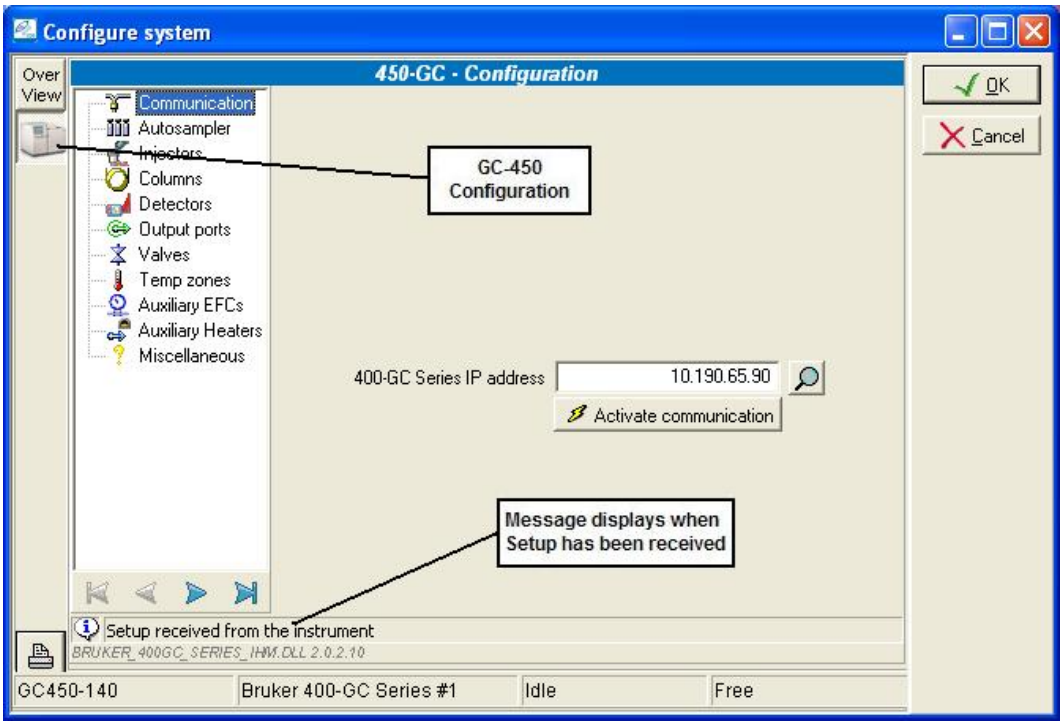
Click on the *Next* button at the bottom of the CompassCDS screens until you obtain the following screen. Click on the *OK* button to configure the system.



The following screen is displayed after you click on *OK*. Click on the *Yes* button.



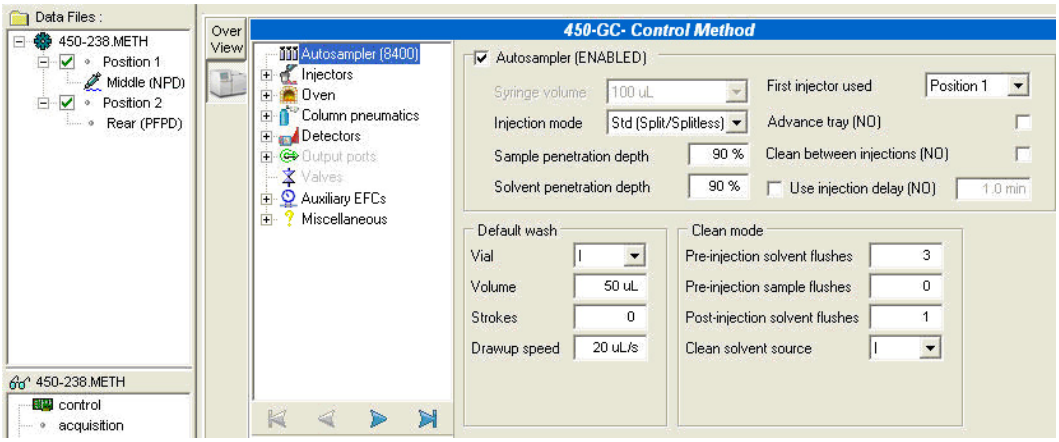
Click on the 400 Series GC Configuration icon and check to make sure that the configuration has been received from the instrument.



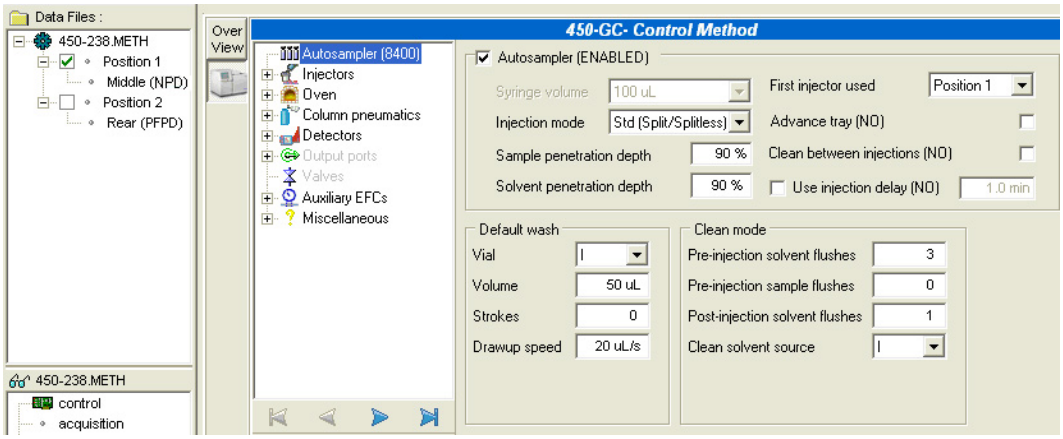
After Setup is uploaded successfully, click on the *OK* button.

You will need to *Start* and *Stop* the instrument before closing the CompassCDS Configuration Manager or before using the system in the CompassCDS software.

After successfully configuring the system in the CompassCDS Configuration Manager, open your instrument in CompassCDS and build a method for it by uploading the method from the instrument. Click on the Data tab at the bottom of the CompassCDS screen and display the method. Click on the AutoSampler selection to show the AutoSampler method. Your screen should look similar to the one displayed below. If you do not see selections for first injector used, Advance tray etc. as displayed in the upper right corner below, then the 400 Series GC is not configured to use both injectors. Go back to the beginning of this document and verify that you have correctly set the 400 Series GC to use both injectors.



Note the left side of the screen above. The expanded tree under the method shows two checkboxes for injectors, front (Position 1) and middle (Position 2). Use these checkboxes to identify which of the two injectors you wish to use in the case that injections into only one injector are required (refer to the CompassCDS manual, *Create a Method* section to see details about the way to use multi-injectors and/or multi-detectors systems).
In the example below the middle injector has been deselected. In this configuration injections will only be made into the front injector.



Refer to the following tables for details about each autosampler parameter.

Parameter	Description
Autosampler	When unchecked, this option allows manual injection and to not use the autosampler (when unchecked, all the sampler parameters become non-active).
Syringe Volume (µL)	Displays the size of the syringe that is installed on the instrument, or the SPME mode. This field is in read only mode.
Injection mode	Consists of five predefined injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile. A sixth User Defined mode is available and allows you access to all autosampler parameters to fine-tune your injection.
Sample penetration depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent penetration depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
First injector used	Corresponds to the injector used for sample injection. If the autosampler is physically mounted in the Front position, position 1 will correspond to the front injector and position 2 will correspond to the middle injector. If the autosampler is physically mounted in the Rear position, position 1 will correspond to the middle injector and position 2 will correspond to the rear injector.
Advance tray	When checked, this option allows injection from two successive vials in the two injectors (**Dual Injection mode**). When unchecked, the sampler will inject from the same vial in the two injectors (**Duplicate Injection mode**).
Clean between injection	When checked, the sampler will perform a wash program before the injection from the second vial.
Use injection delay	Check this option to define a time delay before the injection from the second vial (note: between two injections, without setting an injection delay, the sampler takes about 0.7 minutes).

NOTE: If opening a method created on a system configured with a syringe volume (X µL), on a system fitted out with a different syringe volume (Y µL), an Update button is displayed near the Syringe Volume field. Clicking on this button will reset all the parameters that depend on the syringe volume to the default actual ones. Moreover, a message is displayed on the bottom of the screen to inform the user that the syringe size has changed

NOTES:

- The standard mode is the default and typically yields good results in most applications.

- The volatile sampling mode is used for sampling solvents with high vapor pressures at room temperature.

- The neat sampling mode is used for pure samples requiring minimum contamination with wash solvent (this mode does not use a solvent plug).

- The viscous sampling mode is used for samples with a higher viscosity than water.

- Enter the same number of vials for each injector (*Vial* field in the *Acquisition* method section). The number of the vial injected is displayed on the run log of the chromatogram (acquisition part)

Default wash parameter group

In the Default wash fields, define the parameters that will be used during the default cleaning, which is used in the case that automation is stopped or a serious fault is detected.

Parameter	Description
Vial	Specifies which of the three solvent vials will be used by the default cleaning.
Volume (µL)	Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Drawup speed (µL/s)	Specifies speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

Clean mode parameter group

In the Clean mode fields, define the pre-injection and post-injection syringe clean modes.

Parameter	Description
Pre-injection solvent flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample, before injection.
Pre-injection sample flushes	Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.
Post-injection solvent flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified), after injection.
Clean solvent source	Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.

Internal standard parameter group

This parameter group is displayed when one of the following injection modes is selected: Viscous, Volatile, or User-defined.

If the Use internal standard option is checked, an internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.

Parameter	Description
Vial	Selects which solvent vial contains the internal standard.
Volume (µL)	Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup speed (µL/s)	Specifies the speed at which the internal standard will be drawn up into the syringe.
Pause time	Defines how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap between the internal standard and the sample

NOTE: When this mode of injection is selected, beware that the total volume (volume of sample injected, entered in the Volume field of the Acquisition method section + Volume of internal standard + volume of any air gaps) does not exceed the maximum syringe volume or the autosampler will be faulted and the GC will stay in the Waiting for injection state.

User defined parameter group

When the User defined injection mode has been selected, another parameter group is displayed and allows you to define the general, solvent plug, and viscosity parameters:

User defined parameters

Parameter	Description
Fill volume (µL)	Specifies the sample volume that will be used for each fill stroke.
Fill strokes	Specifies the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.
Sample air gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the sample plug.
Air plug after sample	Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

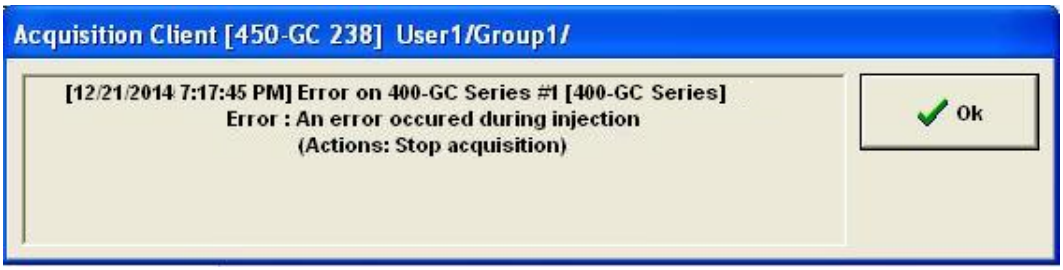
Solvent plug parameters

Parameter	Description
Vial	Selects which solvent vial to use for the solvent plug.
Volume (µL)	Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup speed (µL/s)	Specifies the speed at which the solvent will be drawn up into the syringe.
Pause time	Defines how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the solvent plug.

Viscosity parameters

Parameter	Description
Viscosity delay (sec)	Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Plunger fill speed (µL/sec)	Specifies the speed at which the sample will be drawn up into the syringe.
Plunger inject speed (µL/sec)	Specifies the speed at which the contents of the syringe will be expelled into the injector.
Pre-injection delay (sec)	Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.
Post-injection delay (sec)	Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

NOTE: When a vial is missing, the following message appears:


Acquisition Client [450-GC 238] User1/Group1/
[12/21/2014 7:17:45 PM] Error on 400-GC Series #1 [400-GC Series]
Error : An error occured during injection
(Actions: Stop acquisition)
Ok

Warning message when a vial is missing.

Default settings for predefined autosampler mode

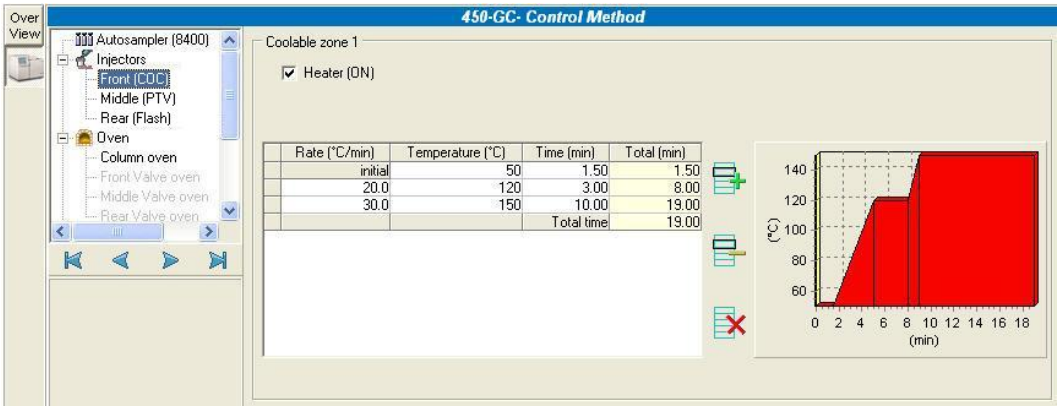
The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

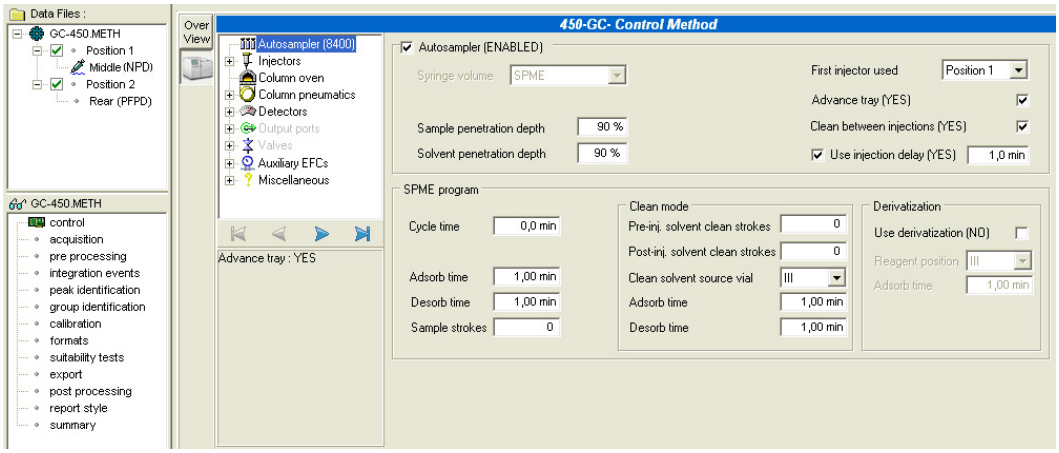
Parameter	Std Split/ Splitless	Std On-Column	Neat [1]	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, you must use User Defined mode.				
PreDefined Settings:					
Fill Volume	10.0 µL	10.0 µL	10.0	Not used	Not used
Fill Strokes	5	5	6	0	0
Sample Air Gap	No	No	No	No	No
Air Plug after Sample	1.0 µL	1.0 µL	1.0 µL	1.0 µL	1.0 µL
Viscosity Settings:					
Viscosity Delay	0.0 sec	0.0 sec	0.0 sec	6 sec	9.9 sec
Plunger Fill Speed	2.0 µL/sec	2.0 µL/sec	2.0 µL/sec	1.0 µL/sec	1.0 µL/sec
Plunger Inject Speed	50 µL/sec	2 µL/sec	50 µL/sec	1 µL/sec	5 µL/sec
Pre-Injection Delay	0.0 sec	0.0 sec	0.0 sec	0.0 sec	0.0 sec
Post-Injection Delay	0.0 sec	6.0 sec	0.0 sec	0.0 sec	12.0 sec

[1] Instead of fill strokes, Neat mode fills the syringe with sample at 2 µL/sec then expels it into the waste cup at 50 µL/sec. It does this a total of six times. Then it fills the syringe with sample at 2 µL/sec and expels it back into the sample vial at 50 µL/sec. This “pumping” action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.

SPME Mode

Refer to the following tables to see details about each autosampler parameter.





Parameter	Description
Autosampler	When unchecked, this option allows you to inject manually and to not use the autosampler (when unchecked, all the sampler parameters become non-active).
Sample penetration depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent penetration depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
First injector used	Corresponds to the injector used for sample injection. If the autosampler is physically mounted in the Front position, position 1 will correspond to the front injector and position 2 will correspond to the middle injector. If the autosampler is physically mounted in the Rear position, position 1 will correspond to the middle injector and position 2 will correspond to the rear injector.
Advance tray	When checked, this option allows injection from two successive vials in the two injectors (**Dual Injection mode**). When unchecked, the sampler will inject from the same vial in the two injectors (**Duplicate Injection mode**).
Clean between injection	When checked, the sampler will perform a wash program before the injection from the second vial.
Use injection delay	Check this option to define a time delay before the injection from the second vial (Note: between two injections, without setting an injection delay, the sampler takes about 0.7 minutes).

NOTE: Enter the same number of vials for each injector (*Vial* field in the *Acquisition* method section). The number of the vial injected is displayed on the run log of the chromatogram (acquisition part).

SPME Program parameter group

In the SPME Program fields, define the parameters that will be used during the SPME.

Parameter	Description
Cycle Time	Specifies the total time of an analysis. This parameter is required only if prep-ahead is used. When using prep-ahead, the prep-vial parameter in the sequence should be set to 2 for this driver.
Adsorb Time	Specifies the time the fiber will stay in the vial.
Desorb Time	Specifies the time the fiber will be exposed in the injector to desorb the sample.
Sample Stroke	Specifies how many times the adsorb time will be repeated before injection.

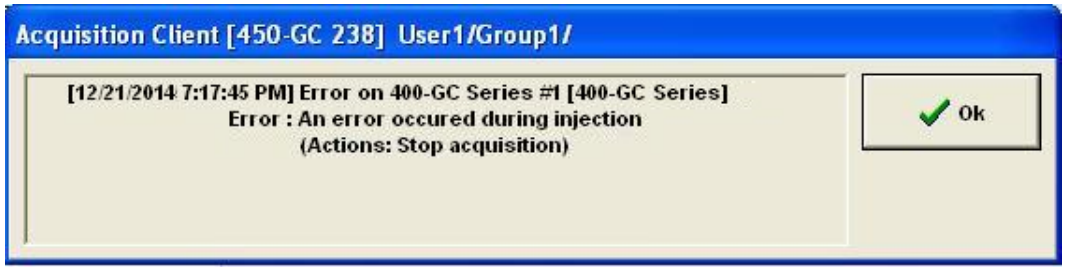
Clean Mode parameters

Parameter	Description
Pre-injection solvent clean strokes	Specifies the number of times the fiber will be cleaned before the injection.
Post-injection solvent clean strokes	Specifies the number of times the fiber will be cleaned after the injection.
Clean solvent source vial	Specifies the clean solvent source vial.
Adsorb time	Specifies the time the fiber will stay in the clean solvent source vial.
Desorb time	Specifies the desorb time during the cleaning cycle.

Derivatization parameters

Parameter	Description
Use derivatization	Specifies if derivatization will be used.
Reagent Position	Specifies the reagent vial.
Adsorb time	Specifies the time the fiber will stay in the reagent vial.

NOTE: When a vial is missing, the following message appears.


Acquisition Client [450-GC 238] User1/Group1/
[12/21/2014 7:17:45 PM] Error on 400-GC Series #1 [400-GC Series]
Error : An error occured during injection
(Actions: Stop acquisition)
Ok

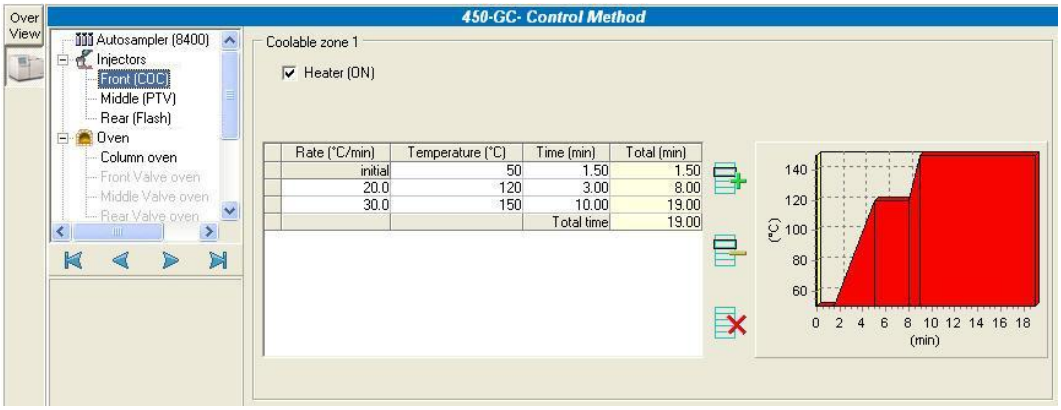
Warning message when a vial is missing.

Injectors Control

The Injectors sub-section contains up to three injectors: Front, Middle, and Rear. Click on the injector you want to edit.

Depending of the system configuration, an injector can be connected to a heat-only zone or to a coolable zone with the coolant activated or not. In these cases, the screens displayed are not exactly the same.

PTV Injector



Coolable zone or Heat-only zone parameter group

Check (or uncheck) the *Heater* option to indicate whether or not you will use the installed injector.

If the injector is connected to a coolable zone and if the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the

injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the injector. The first row of the table contains the initial temperature and hold time for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate (°C/min)* and the *Time* the inlet heater is held at this temperature in the corresponding columns.

NOTE: The graph shows the inlet temperature programming.

Split event table parameter group

If the injector is connected to a Type 21 EFC, you can build a split ratio time program by using the split event table.

The first row of the table contains the *Initial Split state* and *Split ratio* for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed.

The rest of the table contains the time-programmed settings for the injector *Split ratio.* The split valve will be switched to the ratio in each row at the indicated time. If the *Split state* is ON, then the sample is split according to the split ratio specified in the corresponding column. If the state is OFF, all the sample enters the column. The split ratio is defined as the column flow plus the split flow, divided by the column flow.

NOTE:
- You must have already configured the Type 21 EFC in the CompassCDS Configuration Manager before you can program the split ratio. Specifically, to build a PTV Split Ratio Program, a Front PTV must have a corresponding Front Type 21 EFC, a Middle PTV must have a corresponding Middle Type 21 EFC, and a Rear PTV must have a corresponding Rear Type 21 EFC.

- You can use a split ratio of 100 after injection to vent the injector of any residual solvent.

- Use a very low split ratio after flushing to conserve carrier gas.

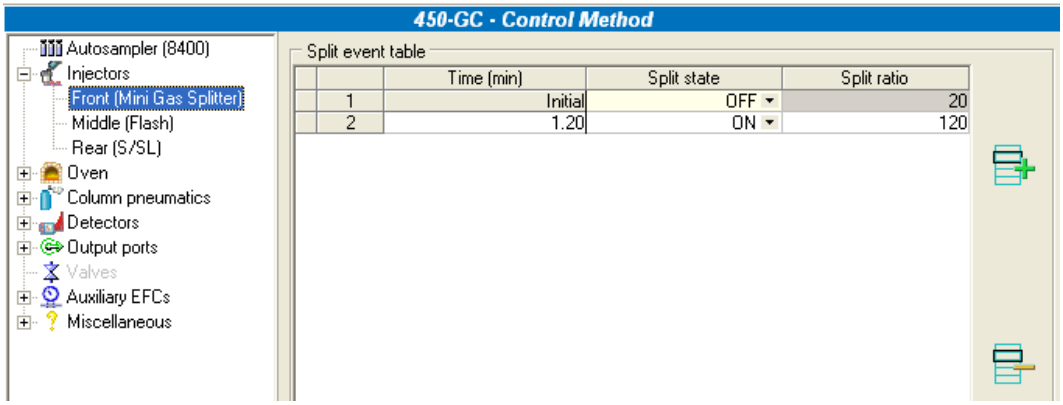
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Mini Gas Splitter



Split event table parameter group

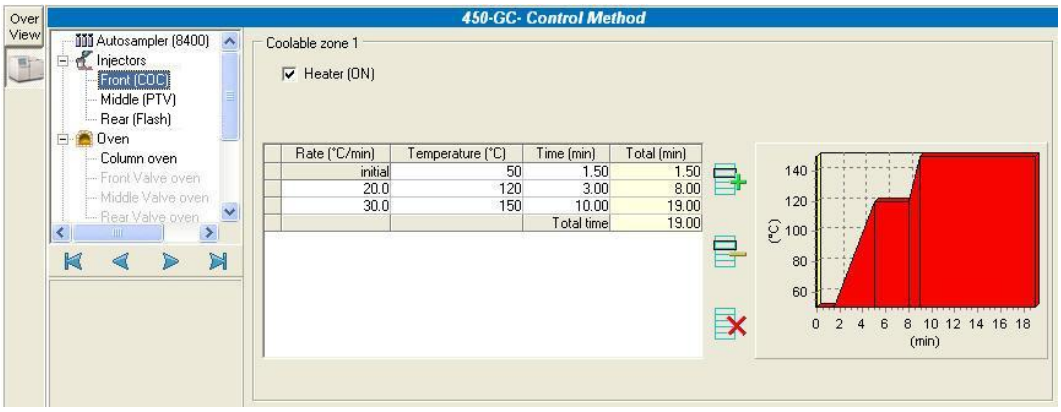
If the injector is connected to a Type 21/25 EFC, you can build a split ratio time program by using the split event table (refer to the PTV injector for more details).

to add a line to the table.

to delete a line in the table.

to clear the entire table.

COC Injector



Coolable zone parameter group

Check (or uncheck) the *Heater* option to indicate whether or not you will use the installed injector.

If the injector is connected to a coolable zone and if the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the injector. The first row of the table contains the initial temperature and hold time for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate (°C/min)* and the *Time* the inlet heater is held at this temperature in the corresponding columns.

NOTE: The graph shows the inlet temperature programming.

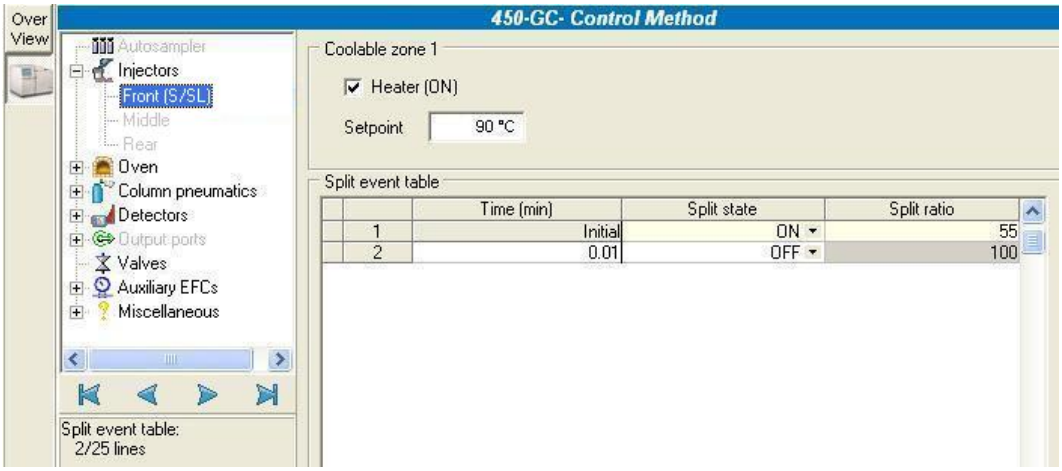
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

S/SL Injector



Coolable zone or Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the *Setpoint* field.

Split event table parameter group

If the injector is connected to a Type 21 EFC, you can build a split ratio time program by using the split event table (refer to the PTV injector for more details).

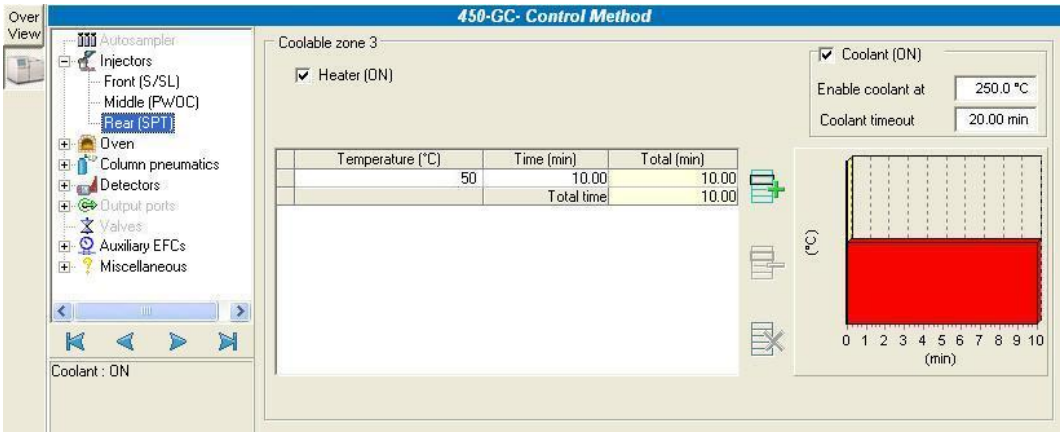
PWOC injector / FLASH injector

Coolable zone or Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the *Setpoint* field.

SPT injector (Sample Preconcentration Trap)



Coolable zone parameter group

Check (or uncheck) the *Heater* option to turn the injector oven ON or OFF.

The SPT must be connected to coolable zone 3. If the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature program to heat and/or cool the injector.

Enter the final temperature of each segment in the *Step* column and the *Time* the inlet heater is held at this temperature in the corresponding column.

Use the following buttons to edit the table:

to add a line to the table.

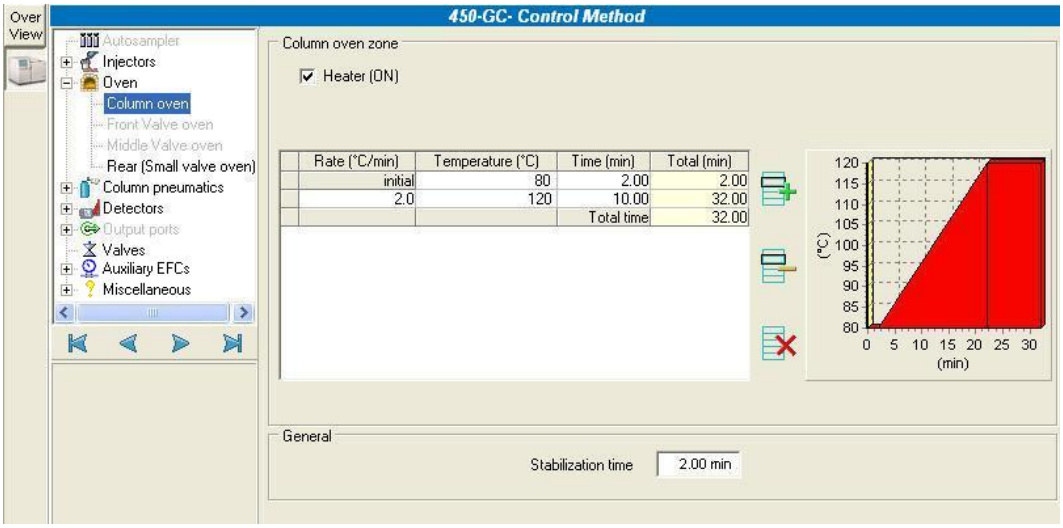
to delete a line in the table.

to clear the entire table.

NOTE: The graph shows the inlet temperature program.

Column Oven Control

The Column oven window contains the column oven program:



Column oven zone parameter group

Check the *Coolant* option if you want to turn the column coolant valve ON. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the column oven fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the column oven.

The first row of the table contains the Initial temperature and hold time for the column oven. The column oven will equilibrate to this setting and stabilize for the specified *Stabilization time* (defined in the **General** parameter group), when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate (°C/min)* and the *Time* the column oven is held at this temperature in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

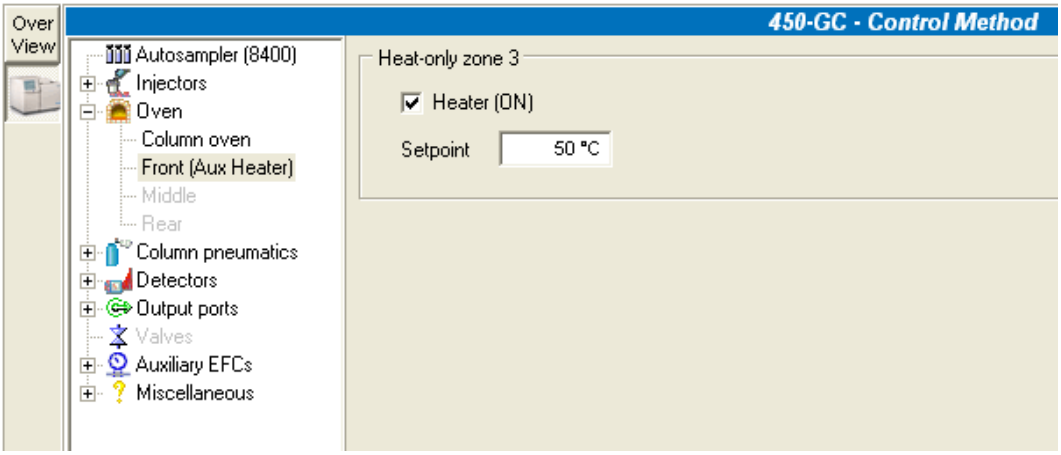
NOTE: The graph shows the column oven temperature program.

General parameter group

Enter the *Stabilization time* in the corresponding field.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

If a valve oven is installed, click on it (Front, Middle or Rear) to display the corresponding window. The valve oven is an optional, isothermal heated zone.



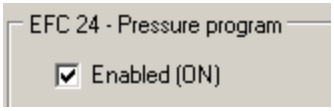
Heat-only zone parameter group

Check (or uncheck) the *Heater* option to indicate whether or not you will use the installed valve.

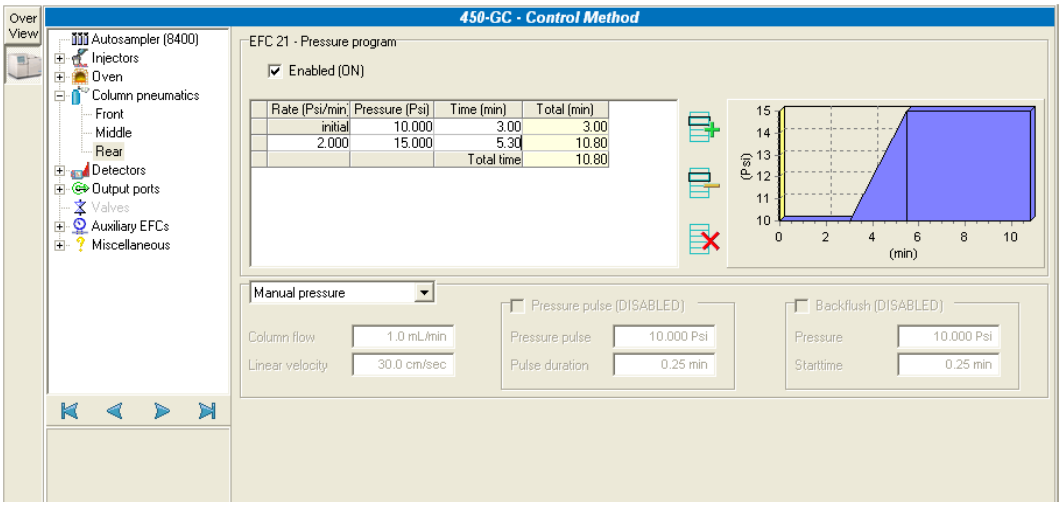
Enter the isothermal temperature of the valve oven in the *Setpoint* field.

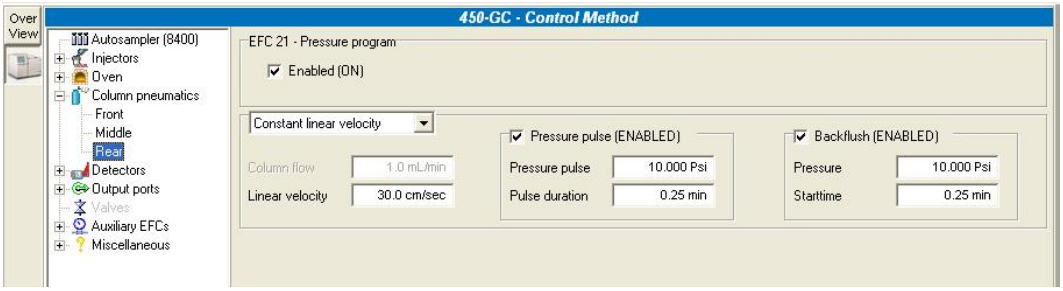
Column Pneumatics Control

The Column pneumatics window contains up to three Electronic Flow Control (EFC) Programs (Front, Middle, Rear). Use the EFC Programs to specify the pressure ramp of the Type 21, Type 22 and Type 25 EFC, the pressure ramp and total flow time program of the Type 24 EFC, and the flow ramp of the Type 23 EFC. All EFCs can be set on and off by clicking the Enabled checkbox.



Type 21 EFC (for PTV/S/SL split/splitless injectors)





NOTE: Type 21 and Type 25 EFCs are identical except with respect to the mechanical plumbing of the pressure sense line. Type 25 EFCs are identified as Type 21 EFCs in software.

Pressure program parameter group

Use the table to build a pressure ramp program.

The first row of the table contains the initial pressure and hold time for the Type 21 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate (Psi/min)* and the *Time* the EPC is held at this pressure in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

NOTE: The graph shows the pressure ramp program.

Pressure mode parameter group

Select *manual pressure* to fill in the pressure table, pressure pulse and backflush are disabled in this mode.

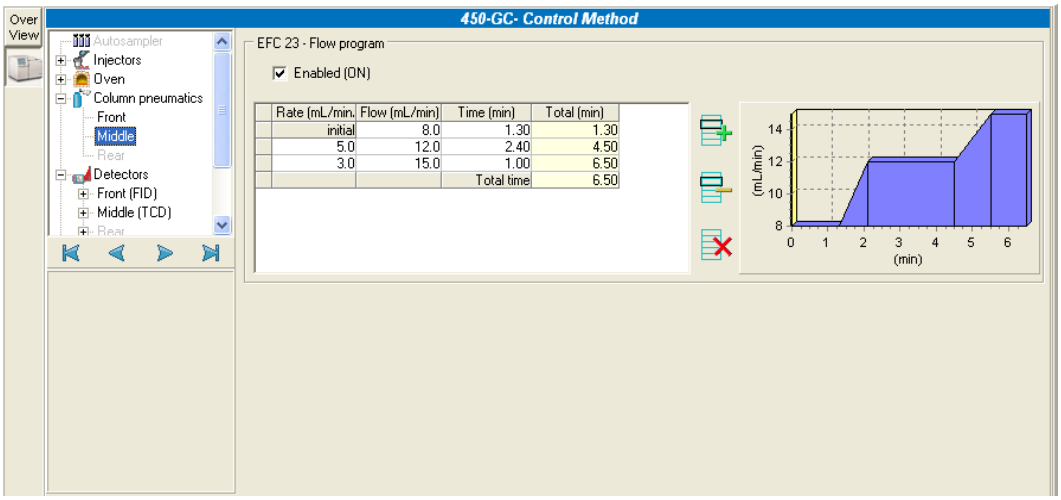
Select *Constant flow* option to disable the table and enter the desired constant *Column flow (mL/min)* in the corresponding field.

Select *Constant Linear velocity* to disable the table and enter the desired constant linear velocity (cm/sec) in the corresponding field.

Check the *Pressure pulse* option to perform a pressure pulse injection. Prior to injection, the pressure will change to the *Pressure pulse* pressure. After injection, the Pressure pulse pressure will be maintained for the *Pulse duration*.

Check the *Backflush* option to perform backflush, refer to the GC User Manual for more information.

Type 23 EFC (for packed columns)



Flow program parameter group

Use the table to build a flow ramp program.

The first row of the table contains the initial flow and hold time for the Type 23 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final flow of each ramp segment in the *Flow* column, the *Rate* (*mL/min/min)* and the *Time* the segment is held at this flow in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

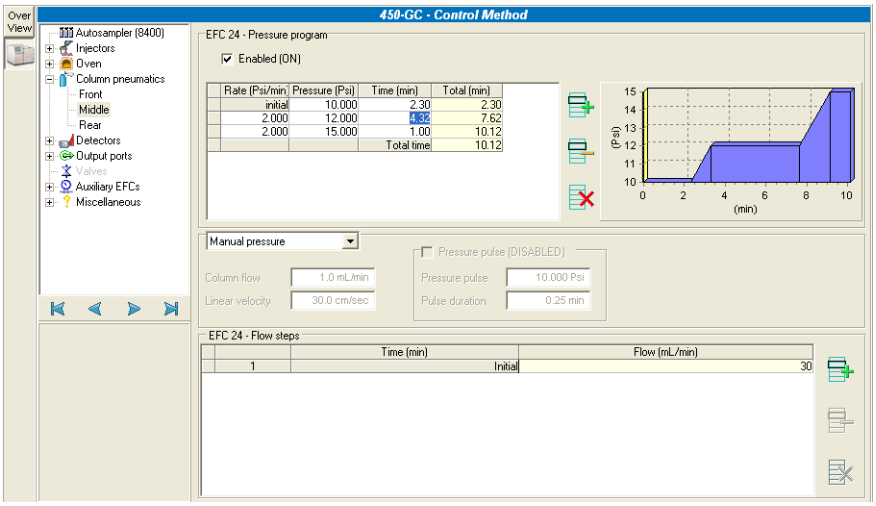
to delete a line in the table.

to clear the entire table.

NOTE: The graph shows the flow ramp program.

Type 24 EFC (for PWOC/FLASH and valved systems)

If a Type 24 EFC is installed, a pressure ramp table and a flow time program table will appear:



Pressure program parameter group

Use the first table to build a pressure ramp program.

The first row of the table contains the initial pressure and hold time for the Type 24 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate (Psi/min)* and the *Time* the EPC is held at this pressure in the corresponding columns.

NOTE: The graph shows the pressure ramp program.

Pressure mode parameter group

Select *manual pressure* to fill in the pressure table, pressure pulse and backflush are disabled in this mode.

Select *Constant flow* option to disable the table and enter the desired constant *Column flow (mL/min)* in the corresponding field.

Select *Constant Linear velocity* to disable the table and enter the desired constant linear velocity (cm/sec) in the corresponding field.

Check the *Pressure pulse* option to perform a pressure pulse injection. Prior to injection, the pressure will change to the *Pressure pulse* pressure. After injection, the Pressure pulse pressure will be maintained for the *Pulse duration*.

Check the *Backflush* option to perform backflush, refer to the GC User Manual for more information.

Flow steps parameter group

Use the second table to build a flow time program to control the Type 24 EFC total flow.

The first row of the flow table contains the initial total flow for the Type 24 EFC.

The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the time-programmed settings for the total flow. The total *Flow* will be switched to the value in each row at the indicated *Time*.

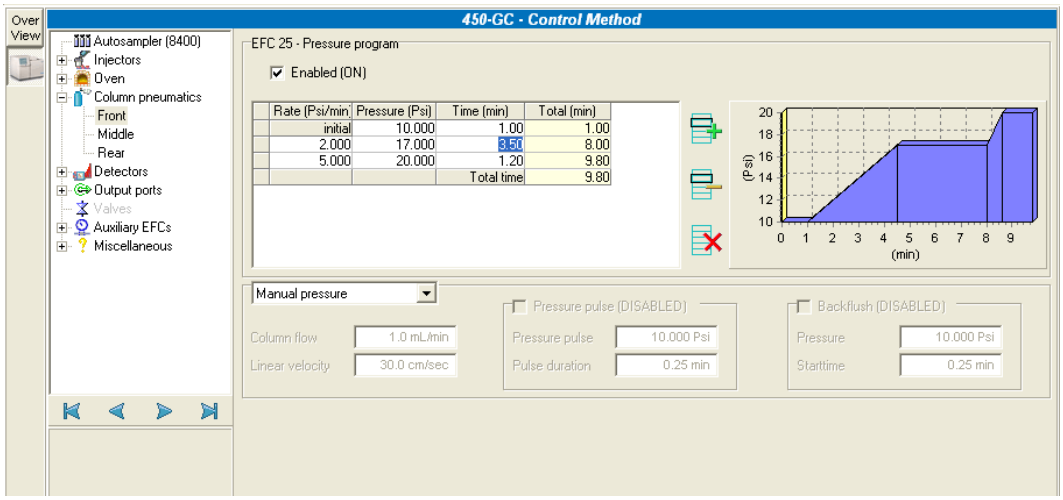
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Type 25 EFC (for PTV and S/SL injectors)



Pressure program parameter group

Use the table to build a pressure ramp program. The first row of the table contains the initial pressure and hold time for the Type 25 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate (Psi/min)* and the *Time* the EPC is held at this pressure in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

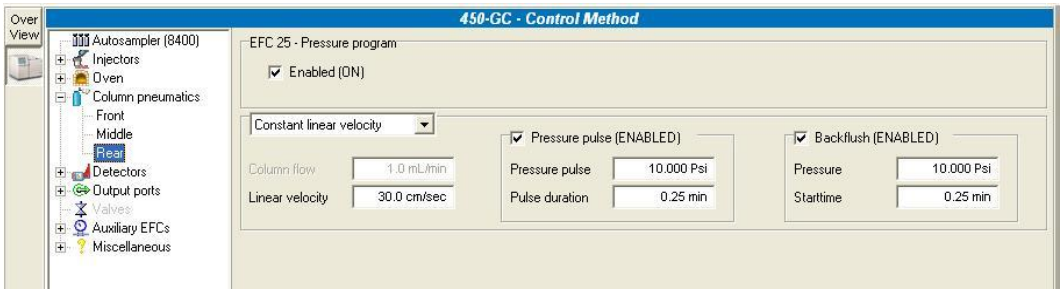
to delete a line in the table.

to clear the entire table.

NOTE: The graph shows the pressure ramp program.

Pressure mode parameter group

Select *manual pressure* to fill in the pressure table, pressure pulse and backflush are disabled in this mode.



Select *Constant flow* option to disable the table and enter the desired constant *Column flow (mL/min)* in the corresponding field.

Select *Constant Linear velocity* to disable the table and enter the desired constant linear velocity (cm/sec) in the corresponding field.

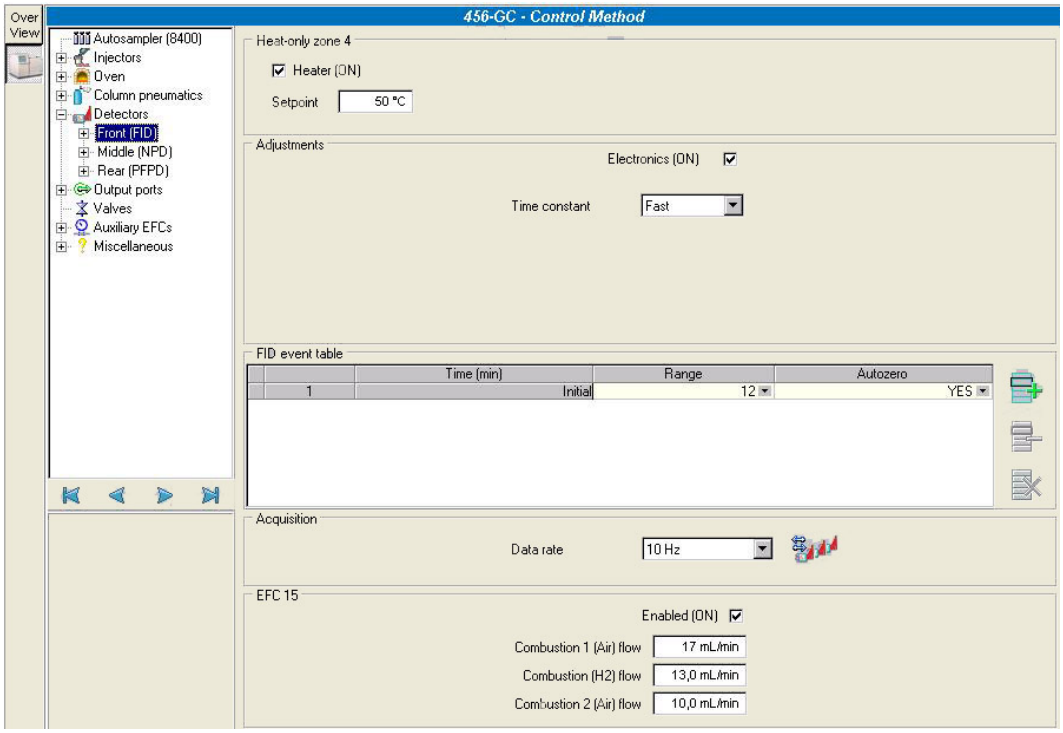
Check the *Pressure pulse* option to perform a pressure pulse injection. Prior to injection, the pressure will change to the *Pressure pulse* pressure. After injection, the Pressure pulse pressure will be maintained for the *Pulse duration*.

Check the *Backflush* option to perform backflush, refer to the GC User Manual for more information.

Detectors Control

The Detectors sub-section contains up to three detectors: Front, Middle, and Rear. Click on the detector you want to edit and specify the operating temperatures, gas flow rates, and specific parameters.

FID Detector (Flame Ionization Detector)



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments parameter group

Check (or uncheck) the *Electronics* option to indicate whether the installed FID will be used or not. Select the required *Time constant* from the list.

FID event table parameter group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range* and *Autozero* for the FID detector. When the initial autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The rest of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Acquisition

Set the detector frequency (Data rate). With the feature Multi Data Frequency Stream it is possible, in combination with a data handling package, to receive data from each detector in a specific frequency.

To use the Multi Data Frequency Stream feature, the AnalogOutput option enable must be unchecked (GC setup; detector tab) only if an option board is installed (GC). If AnalogOutput is used, the detector frequency between all detectors will be synchronized. A synchronization icon will be visible.

NOTE: In combination with an MIB 8x0 box, Multi Data Frequency Stream is not possible.

NOTE: AnalogOutput is disabled by default after installation of the option board. To make use of the Multi Data Frequency Stream feature, the AnalogOutput must remain disabled.

Multi Data Frequency Stream requirements:

- Only available in 436 and 456-GC.
- GC firmware must be version 5.06 or higher.
- Option board installed? Switch off AnalogOutput.
- CompassCDS “400 Series GC” driver must be version 2.0.3.17. or higher.

Type 11 EFC parameter group

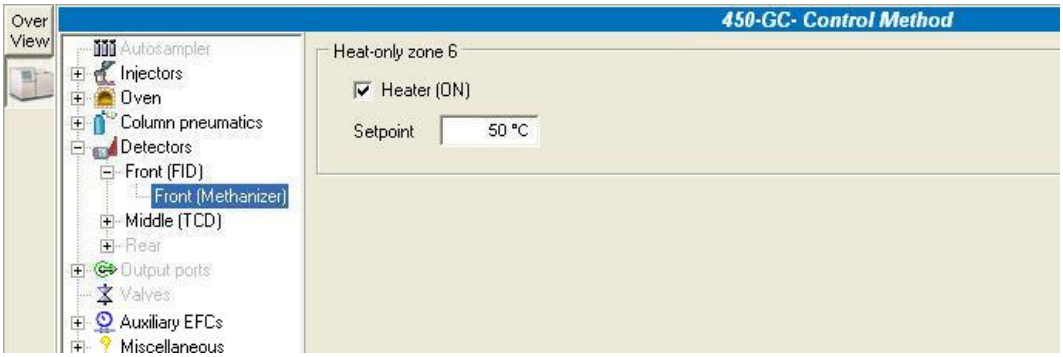
If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and allow you to define the desired gas flow rates I**t is possible to turn the EFC on and off by clicking the Enabled checkbox:**

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For FID detectors, the EFC Type 11 is required.

Methanizer

A methanizer is an option that converts carbon monoxide and carbon dioxide to methane.

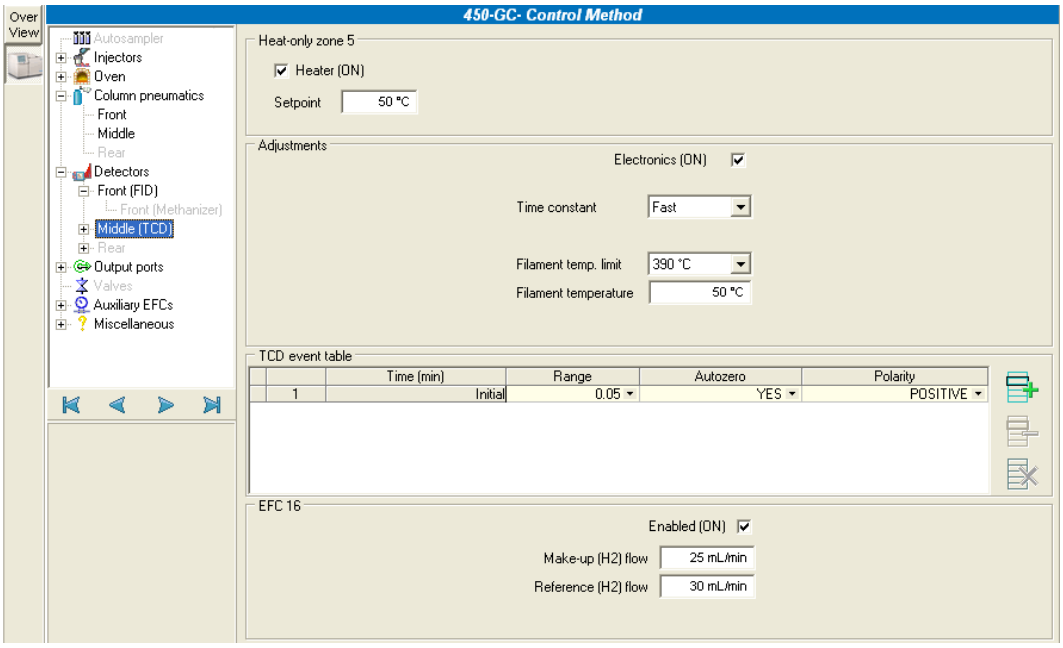
It is associated with a specific FID detector; consequently, it is accessed in the *Detector* section:



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the methanizer oven ON or OFF and enter the methanizer oven temperature in the *Setpoint* field.

TCD Detector (Thermal Conductivity Detector)



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments parameter group

Check (or uncheck) the *Electronics* option to indicate whether the installed TCD will be used or not. Select the required *Time constant* from the list.

Specify the *Filament temperature* in the corresponding field and select the *Filament temperature limit* from the list. To protect the filament, always operate the detector with the 390 °C limit selected unless you require the maximum dynamic range available to the TCD. With the limit set to 390 °C, the peak sample filament temperature is limited to approximately 450 °C. The temperature limit is approximately 550 °C at the 490 °C setting. The 450 °C limit protects filaments from oxidation when exposed to air over an extended period of time. However, at the 550 °C temperature limit the filament can degrade after only a few minutes.

TCD event table parameter group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range*, *Autozero* and *Polarity* for the TCD detector. When the initial autozero is set to yes, it means the detector autozero is on continuously before the run starts. The polarity is used to reverse the peaks that appear in the negative direction (for example, if you inject a standard or sample into the reference side of the TCD).

The rest of the table contains the time-programmed settings: the *Range*, *Autozero* and *Polarity* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

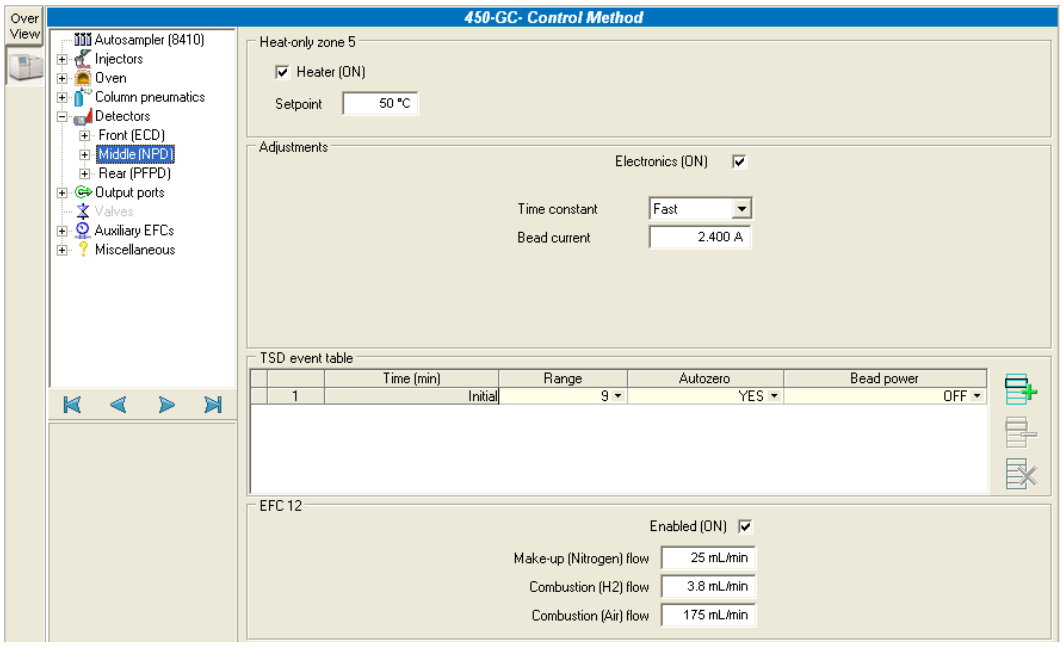
NOTE: In dual TCD detector the heater zone is common for both TCD detectors.

Type XY EFC parameter group for each type of EFC it is possible to turn the EFC on and off by clicking the Enabled checkbox:

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For TCD detectors, three EFC types are available: Type 13, Type 14 and Type 16.

If the detector Electronic Flow Control module is installed, the Type XY EFC section will appear and allows you to define the desired gas make up flow rate.

NPD Detector (Thermionic Specific Detector)



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments parameter group

Select the required *Time constant* from the list.

Specify the *Bead current* (i.e., bead surface temperature) in the corresponding field; it corresponds to the current at which the gas phase chemistry will initiate.

NPD event table parameter group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range*, *Autozero* and *Bead power* state for the NPD detector. When the initial autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The rest of the table contains the time-programmed settings: the *Range*, *Autozero* and *Bead power* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

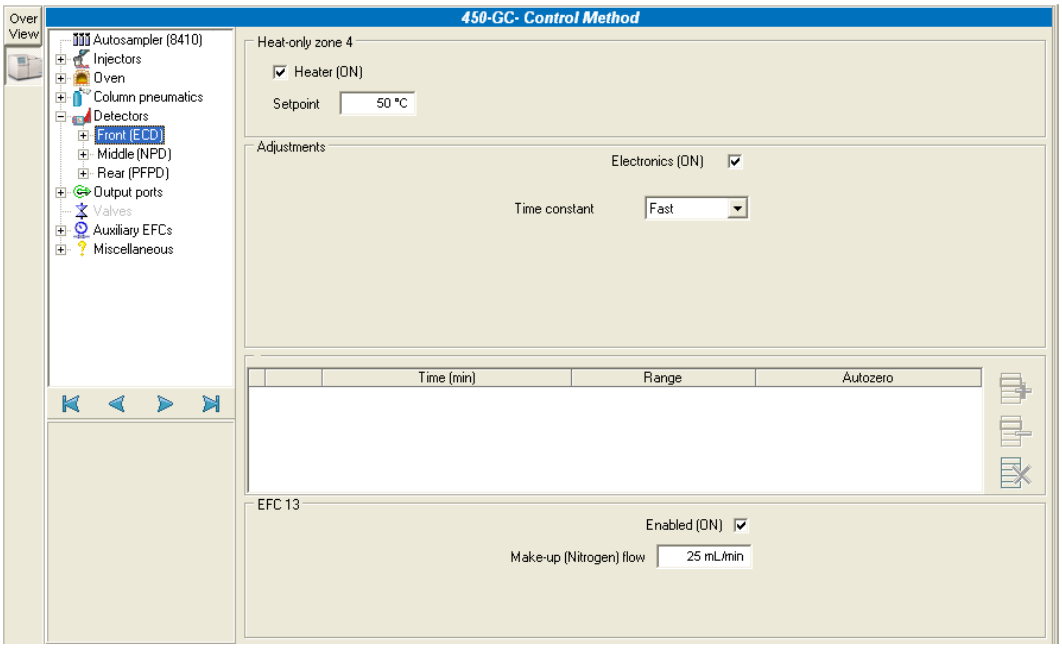
to clear the entire table.

Type 12 EFC parameter group

If the detector Electronic Flow Control module is installed, the Type 12 EFC section will appear and allows you to define the desired gas flow rates. I**t is possible to turn the EFC on and off by clicking the Enabled checkbox:**

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For NPD detectors, the EFC Type 12 is required.

ECD Detector (Electron Capture Detector)



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments parameter group

Check (or uncheck) the *Electronics* option to indicate whether the installed ECD will be used or not.

Select the required *Time constant* from the list. For most applications, select the SLOW setting. For capillary applications with peak widths at half height of less than 2 seconds, select the FAST setting.

Specify the *Cell current* and *Cell contact potential* in the corresponding fields.

The choice of cell current depends on the specific carrier gas that is used and the baseline signal with only carrier gas present. For normal operation with nitrogen carrier gas, use the N2STD or CAP setting. When a greater linear range is desired, select the Ar/CH4 setting and use 90%Argon / 10% Methane as the carrier gas.

ECD event table parameter group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range* and *Autozero* for the ECD detector. When the initial autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The rest of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

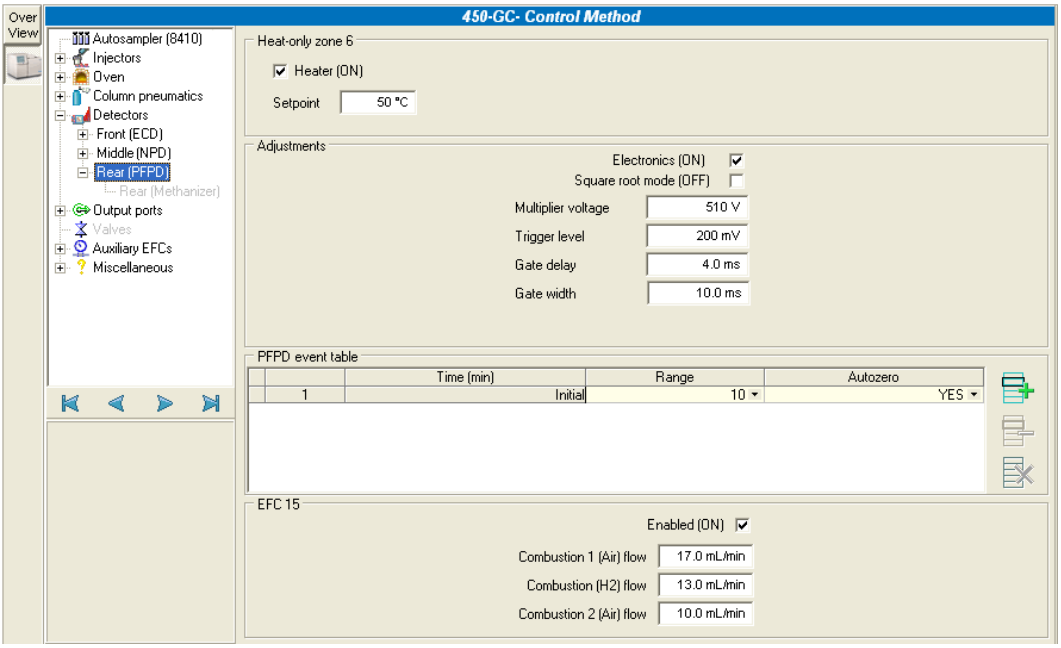
to clear the entire table.

Type 13 EFC parameter group

If the detector Electronic Flow Control module is installed, the Type 13 EFC section will appear and allows you to define the desired gas make-up flow rate. I**t is possible to turn the EFC on and off by clicking the Enabled checkbox:**

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For ECD detectors, the EFC Type 13 is required.

PFPD Detector (Pulsed Flame Photometric Detector)



Heat-only zone parameter group

Check (or uncheck) the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments parameter group

Check (or uncheck) the *Electronics* option to indicate whether the installed PFPD will be used or not.

Check (or uncheck) the *Square root mode* option to enable (or disable) this mode.

Enter the PFPD photomultiplier voltage in the *Tube voltage* field and select the desired *Trigger level*, *Gate delay* and *Gate width* in the corresponding fields.

PFPD event table parameter group

Use the table to change detector settings during the analysis.

The first row of the table contains the *initial Range* and *Autozero* for the PFPD detector. When the initial autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The remainder of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

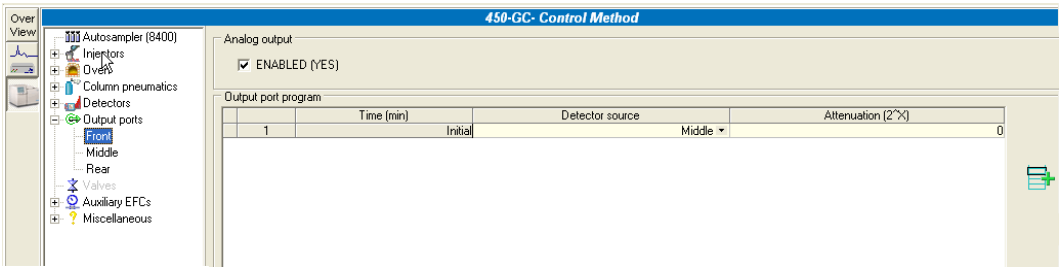
Type 15 EFC parameter group

If the detector Electronic Flow Control module is installed, the Type 15 EFC section will appear and allows you to define the desired gas flow rates. **It is possible to turn the EFC on and off by clicking the Enabled checkbox:**

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For PFPD detectors, the EFC Type 15 is required.

Output Ports Control

The 400 Series GC has three analog output ports, which allow analog data to be sent to external integrators or other analog data systems:



Analog output parameter group

Check (or uncheck) the Enabled option to turn the Analog output ON or OFF.

Output port program parameter group

Use the table to time program the *Detector* signal *source* and *Attenuation* at each port. The first row of the table contains the initial signal *source* and *Attenuation* for the port.

Use the following buttons to edit the table:

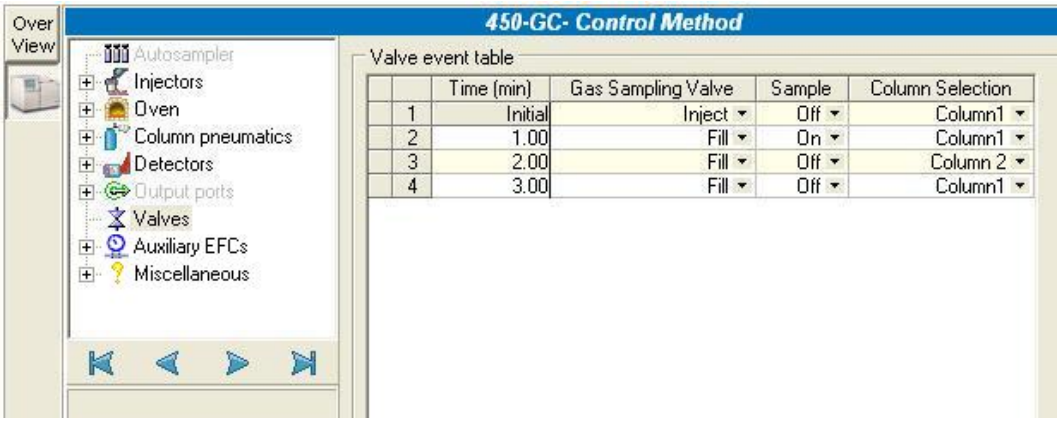
to add a line to the table.

to delete a line in the table.

to clear the entire table.

Valves Control

The 400 Series GC can be configured with a wide variety of valves. The Valves window contains the valves table program (for sample delivery) and up to fifteen valve oven programs:



Valve event table parameter group

Use the table to change valves settings during the analysis.

The first row of the table contains the initial setting for each valve. The rest of the table contains the time-programmed settings: each valve will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

to add a line to the table.

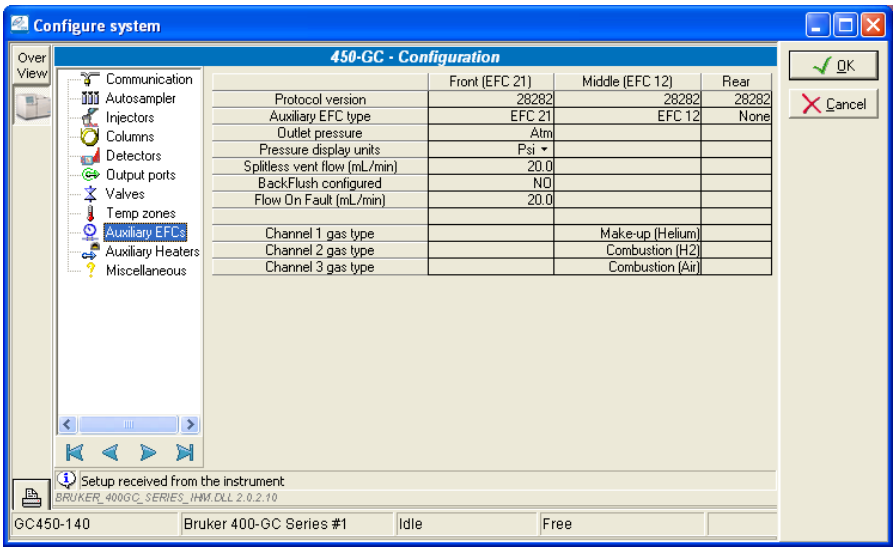
to delete a line in the table.

to clear the entire table.

Valve type	Description
Split valve	Splitless or split The 400 Series GC can have up to three split valves installed (Front, Middle, Rear)
Gas sampling valve	Fill or Inject
Liquid sampling valve	Fill or Inject
Sample	Off or On
Internal standard	Off or On
Surrogate standard	Off or On
Series bypass	Series or Bypass
Backflush to detector	Forward or Backflush
Backflush to vent	Forward or Backflush
Column selection	Column 1 or Column 2
Injection + Backflush to detector	Fill and Backflush or Inject
Injection + Backflush to vent	Fill and Backflush or Inject
Alternate injection	Column 1 or Column 2
Simultaneous injection	Fill or Inject
Methanizer bypass	Series or Bypass
Sample preconcentration trap	SPT desorb or SPT trap
Event A, B, C, D, E, F, G, H, I J	Off or On

Auxiliary EFCs

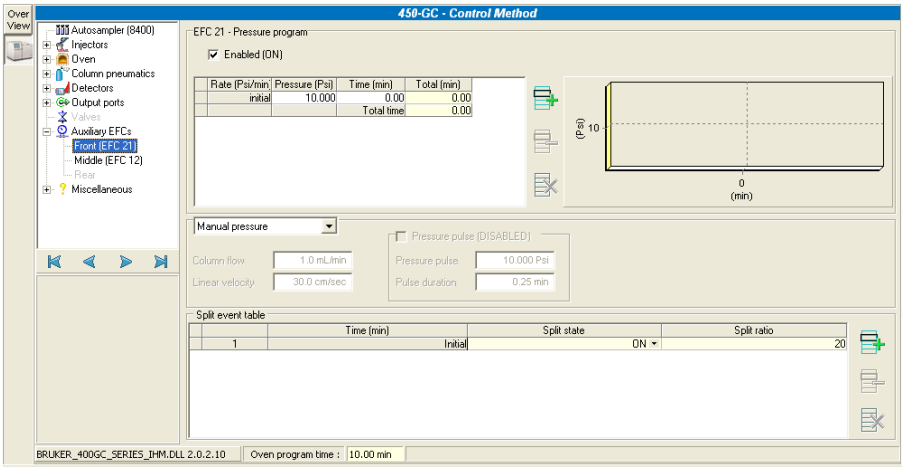
The Auxiliary EFCs window contains parameters for EFCs as a new device.



The EFCs represents al Injector and Detector EFCs and could be placed in front, middle and rear position.

If one or more auxiliary EFCs are configured a synopsis screen will be available for status indication.

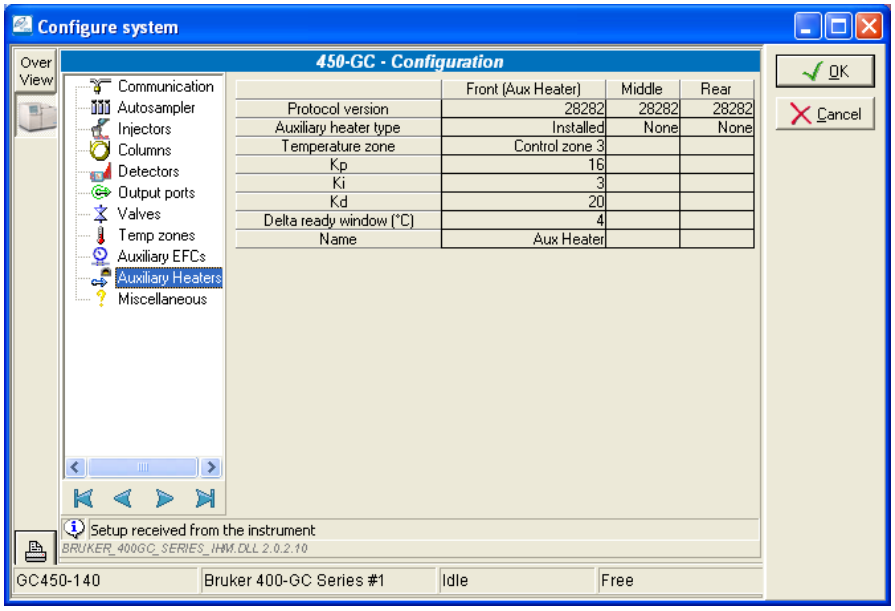
For details about the EFC see *Column Pneumatics Control* and Detectors Control.



Auxiliary Heaters

The Auxiliary Heaters window contains parameters for heated device as a new device.

If one or more auxiliary heater or valve oven is configured, a synopsis screen will be available for status information.



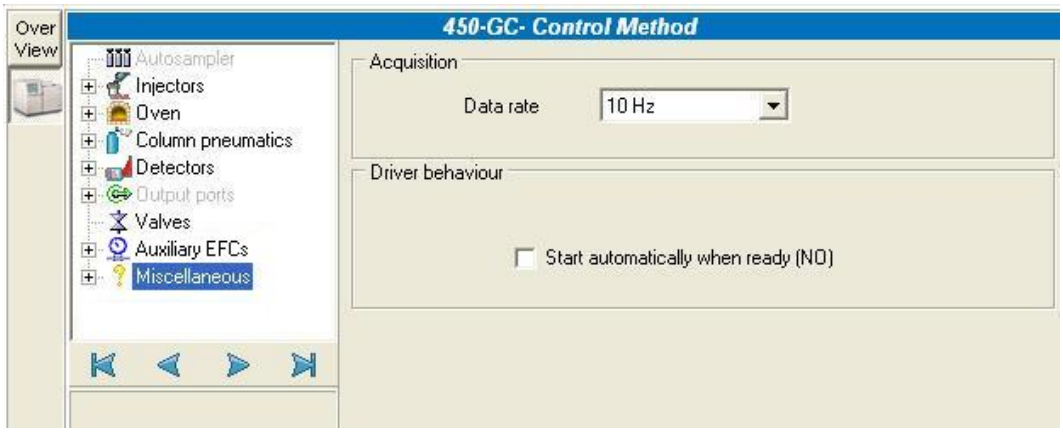
Heat-only zone parameter group

Check (or uncheck) the *Heater* option to indicate whether or not you will use the installed valve.

Enter the isothermal temperature of the Auxiliary Heater in the *Setpoint* field.

Miscellaneous

The Miscellaneous window contains parameters for data collection



Acquisition parameter group

Enter the detector data rate in the *Data rate* field. With decreased data rates, less disk space is required for storing the data. With increased rates, more data is collected, which may improve quantitation, particularly for narrow peaks.

Driver behavior parameter group

Check *Start automatically when ready* to start the GC without injecting. This could be useful in case of sampling valve use, for example.

Starting and Viewing an Acquisition

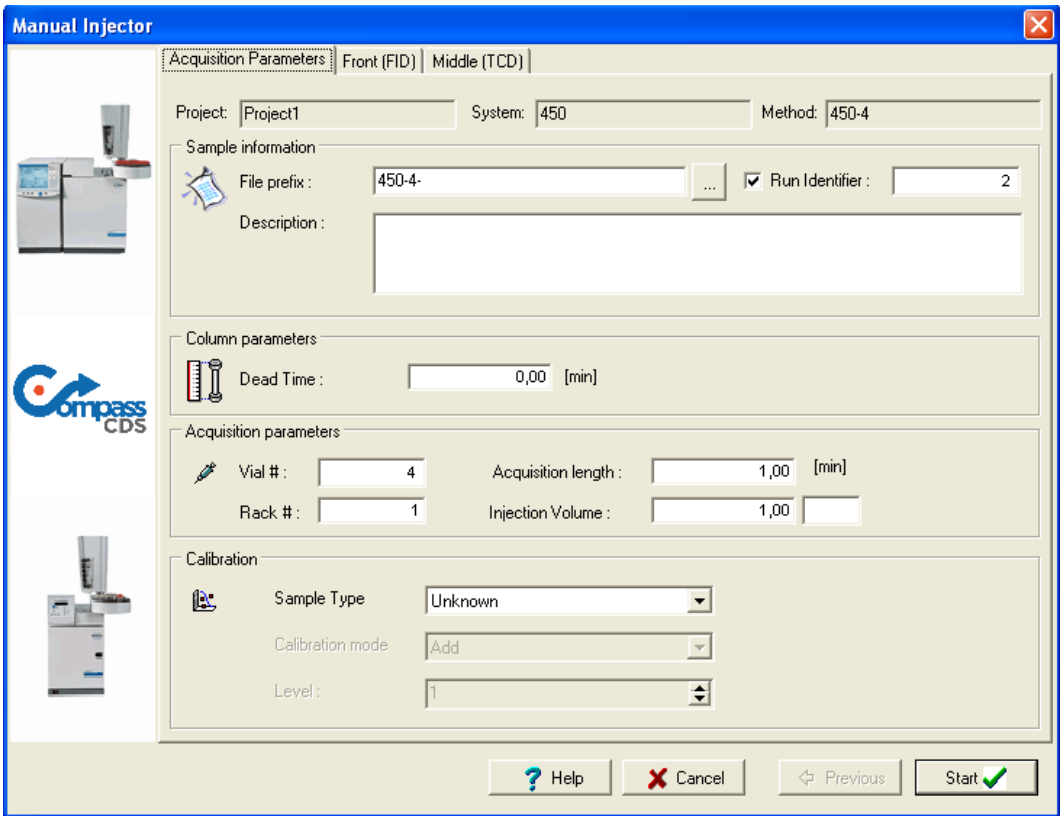
Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

Quick Start (Single Acquisition)

1. Press the button.
2. In the ***Quick Start*** window, select the system, the method and optionally the project if connected in "All project" mode.
3. Press the *OK* button.

The following screen is displayed:



In the *Acquisition parameters* tab, required like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by CompassCDS, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

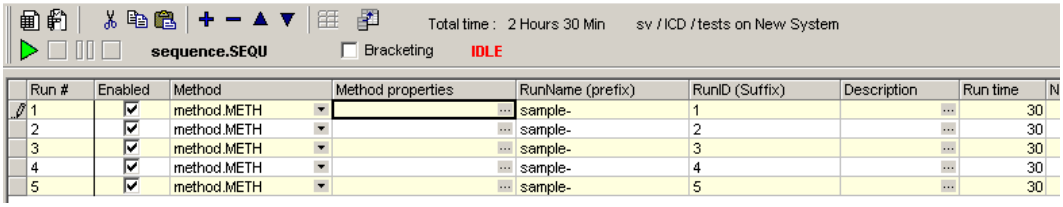
Other parameters associated with each acquisition channel can be entered in the *Channel X* tab.

4. Click on the *Start* button to start the acquisition if the system is a single-injector system or click on the *Next* button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the ***FILE / NEW SEQUENCE*** *menu*, and complete the displayed creation wizard screen (refer to the CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time
1	☑	method.METH		sample-	1		30
2	☑	method.METH		sample-	2		30
3	☑	method.METH		sample-	3		30
4	☑	method.METH		sample-	4		30
5	☑	method.METH		sample-	5		30

The *Method Name*, the *Run Name*, the *Run ID,* and the *Acquisition length* must be filled before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the 400 Series GC

Click on the button corresponding to the 400 Series GC driver and the status screen will appear. It contains nine sub-sections: *Autosampler*, *Injectors*, *Column oven*, *Columns*, *Detectors*, *Output ports*, *Valves*, *Miscellaneous*, and *Overview*. Click on the required sub-section to display the corresponding parameters that will be used during the chromatographic run.

A toolbar allows you to easily scroll through the status windows:

to select the first status window.

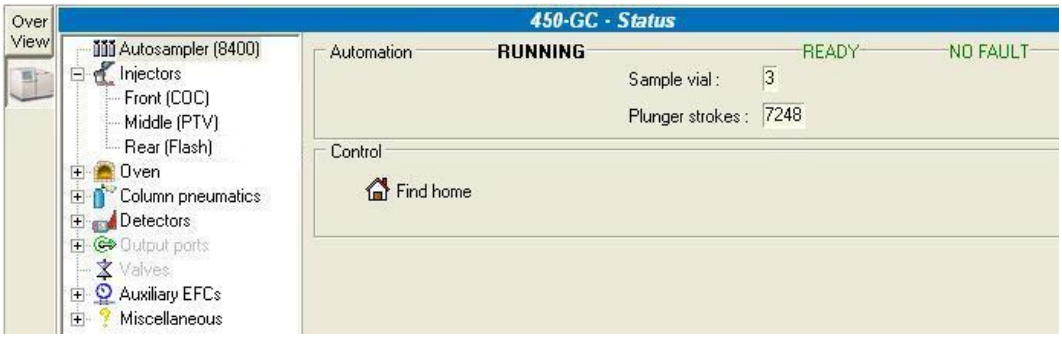
to move back to the previous status window.

to move forward to the next status window.

to select the final status window.

Autosampler Window

This option is only shown on 400 Series GC that have an 8400 AutoSampler or 8410 AutoInjector connected to them.



The Autosampler status screen indicates the autosampler state (Ready, Running, Suspended, Resetting or Running Priority Sample).

The display also includes the following parameters:

Sample vial: Corresponds to the current vial.

Plunger Strokes: Displays the number of times that the syringe plunger has been stroked up and down. This can be used to help monitor syringe wear and plan for syringe replacement.

Present: Indicates whether the tray is present or not.

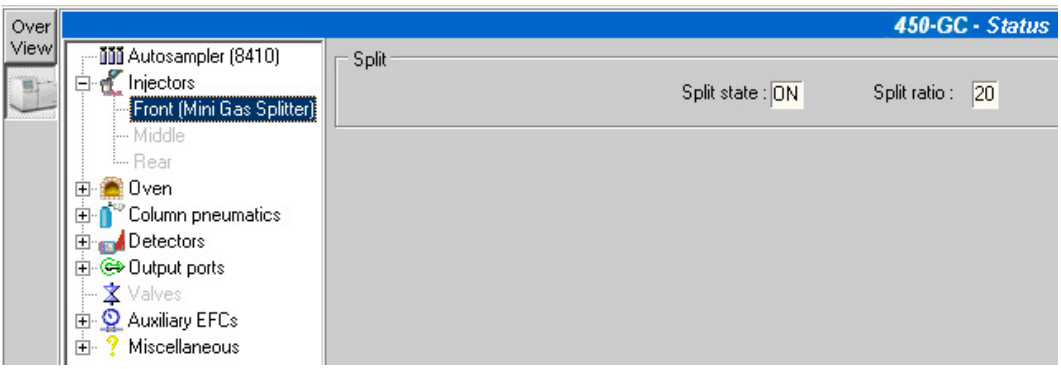
Orientation: Shows the range of vials accessible from the carrousel location (8410 AutoInjector Only)

Click on the

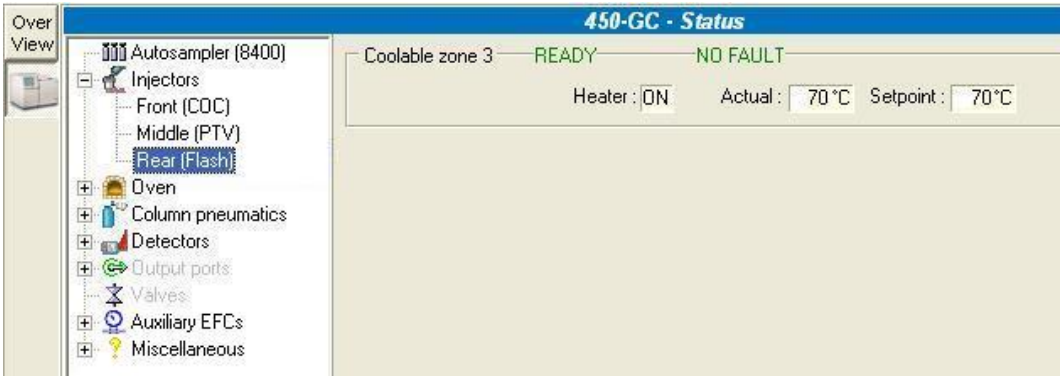
button to reinitialize the autosampler.

Mini Gas Splitter Window

This option is only shown on a 400 Series GC that have a Mini Gas Splitter.



Injectors Window



The following status parameters are available for any injector type:

Ready, *Not ready or OFF*: The injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance. The injector oven is OFF when the heater is OFF.

Fault or *No Fault*: Displays if a fault in the injector component has occurred.

Heater: Displays if the injector oven component is turned OFF or ON at the 400 Series GC.

Actual: Displays the actual temperature of the injector oven at the 400 Series GC.

Setpoint: Displays the injector oven programmed temperature setting in the active method.

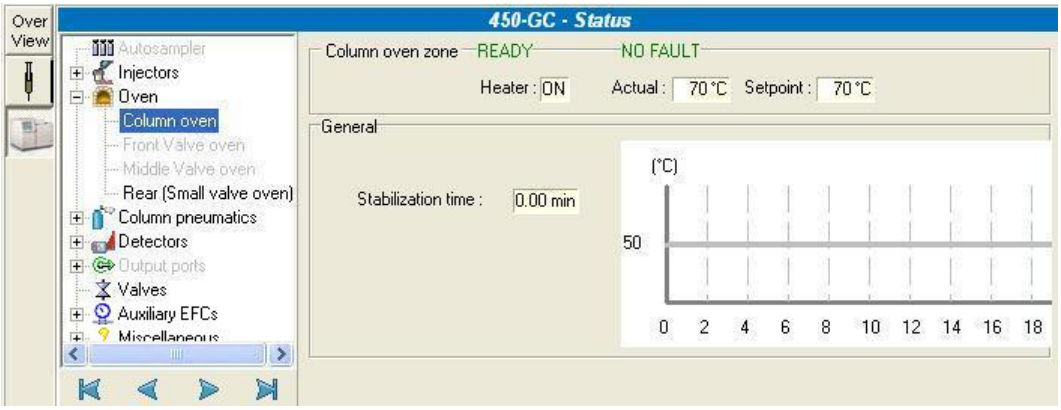
NOTE: The Mini Gas Sampler injector does not have the heating parameters.

Other parameters can be displayed according to the injector type:

Injector	Parameter	Description
PTV	Coolant enable	displays if the PTV injector oven coolant is enabled in the active method.
	Timeout period	displays the programmed coolant time-out value in the active method for the PTV injector oven. The countdown begin as soon the temperature is reached and injector turns to ready. GC is turned on standby as soon as the countdown is finished.
	Threshold	displays the programmed injector oven temperature at which the PTV injector oven coolant is enabled.
	Split state	displays the current split state of the PTV injector method.
	Split ratio	displays the current split ratio of the PTV injector method. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.
S/SL	Split state	displays the current split state of the S/SL injector method.
	Split ratio	displays the current split ratio of the S/SL injector method. The split ratio is defined as the (Column Flow + Split Flow) / the Column Flow.
SPT	Coolant enable	displays if the SPT injector oven coolant is enabled in the active method.

Injector	Parameter	Description
	Threshold	displays the programmed injector oven temperature at which the SPT injector oven coolant is enabled.
	Timeout period	displays the programmed coolant time-out value in the active method for the SPT injector oven.
MGS	Split state	displays the current split state of the MGS injector method.
	Split ratio	displays the current split ratio of the MGS injector method. The split ratio is defined as the (Column Flow + Split Flow) / the Column Flow.

Oven Window Column Oven



The status displays includes the following parameters:

Ready, *Not Ready or OFF:* The column oven is Ready if the setpoints have been achieved and stabilized. The column oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance. The column oven is OFF when the Heater is turned OFF.

NOTE: Some reasons the GC may go Not Ready during a run are: the temperature program is too aggressive, the oven door is opened, the coolant runs out, the power line voltage drops, etc.

Fault or No Fault: Displays if a fault in the column oven component has occurred.

Heater: Displays if the column oven component is turned OFF or ON at the 400 Series GC.

Actual: Displays the actual temperature of the column oven at the 400 Series GC.

Setpoint: Displays the column oven programmed temperature setting in the active method.

The graph of Column oven program is displayed.

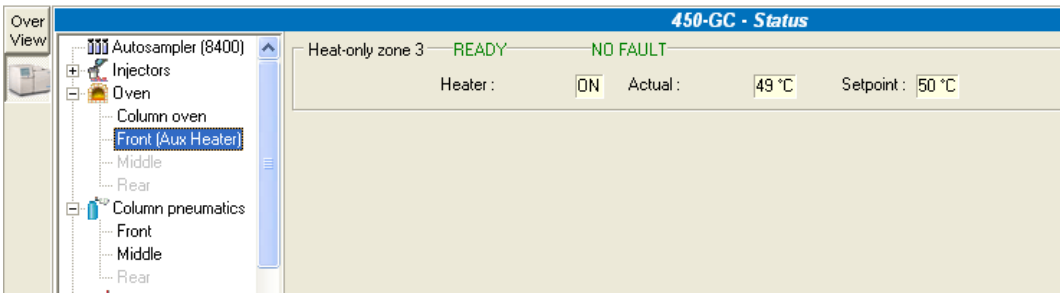
Coolant enable: Displays if the column oven coolant is enabled in the active method.

Threshold: Displays the programmed column oven temperature at which the column oven coolant is enabled.

Timeout period: Displays the programmed coolant time-out value in the active method for the column oven.

Stabilization time: Shows the 400 Series GC column oven stabilization time in minutes. The stabilization time counts down from the programmed method value and then displays 0.00 minutes when the stabilization period is over.

Oven Window Auxiliary Heater



The status display includes the following parameters:

Ready, *Not Ready or OFF:* The Aux. heater is Ready if the setpoint have been achieved and stabilized. The Aux. heater is Not Ready if readiness to start a run has not been achieved or if, during a run, the Aux. heater becomes not ready or goes out of tolerance. The Aux. heater is OFF when the heater is turned OFF.

Fault or No Fault: Displays if a fault in the Aux. heater component has occurred.

Heater: Displays if the Aux. heater component is turned OFF or ON at the 400 Series GC.

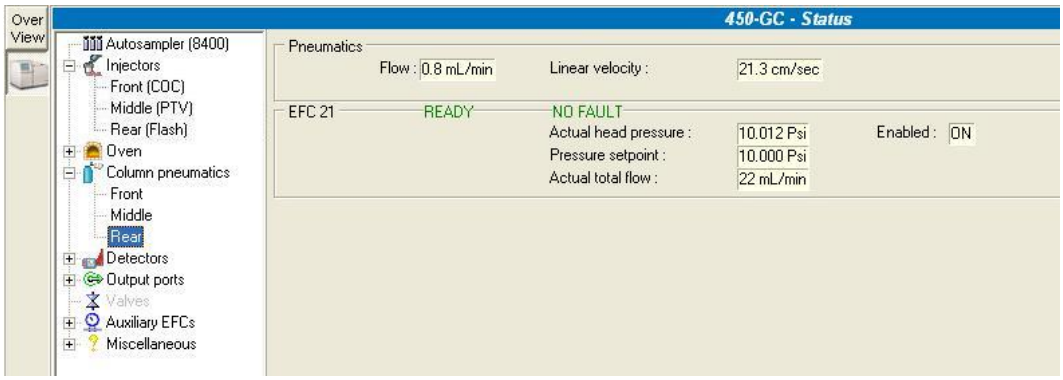
Actual: Displays the actual temperature of the Aux. heater at the 400 Series GC.

Setpoint: Displays the Aux. heater isotherm temperature setting in the active method.

Column Pneumatics window

The columns status screen depends on the installed EFC modules.

Type 21 EFC Status screen



The status display includes the following parameters:

Ready or *Not Ready*: The Type 21 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 1 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

Fault or *No Fault*: Displays if a fault in the Type 21 EFC component has occurred.

Flow: Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

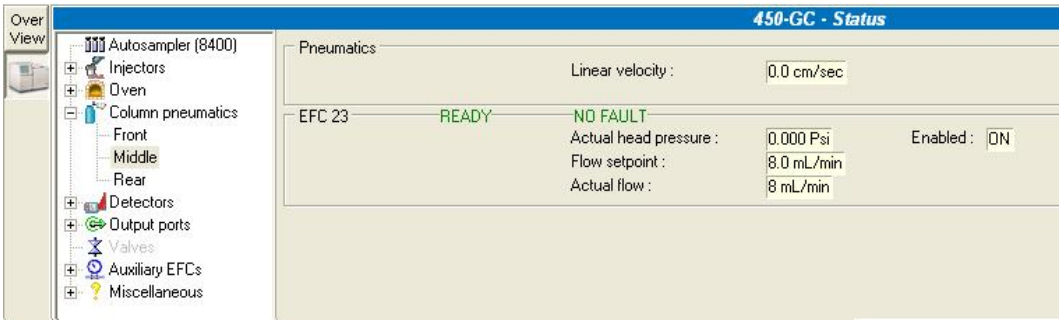
Linear velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual head pressure: Displays the actual column head pressure at the 400 Series GC.

Pressure setpoint: Displays the programmed column head pressure setting in the active method.

Actual total flow: Displays, in mL/min, the total flow rate through the system.

Type 23 EFC Status screen



The status display includes the following parameters:

Ready or *Not Ready*: The Type 23 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 23 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

Fault or *No Fault*: Displays if a fault in the Type 23 EFC component has occurred.

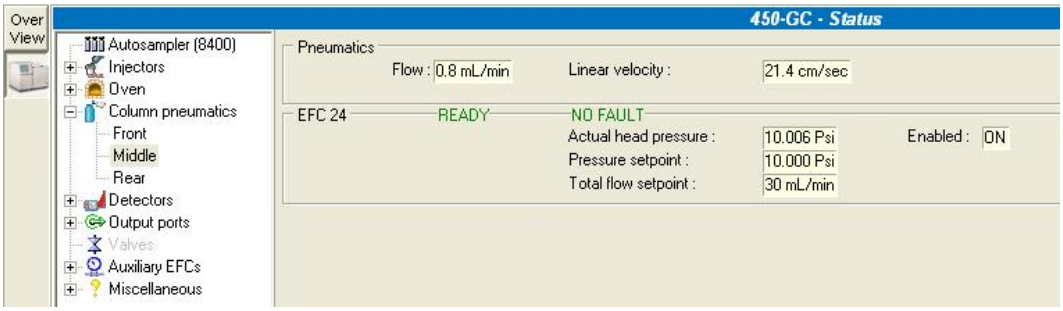
Linear velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual head pressure: Displays the measured column head pressure at the 400 Series GC.

Total flow setpoint: Displays the programmed total flow rate setting in the active method.

Actual flow: Displays, in mL/min, the actual total flow rate.

Type 24 EFC Status screen



The status display includes the following parameters:

Ready or *Not Ready*: The Type 24 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 24 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

Fault or *No Fault*: Displays if a fault in the Type 24 EFC component has occurred.

Flow: Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

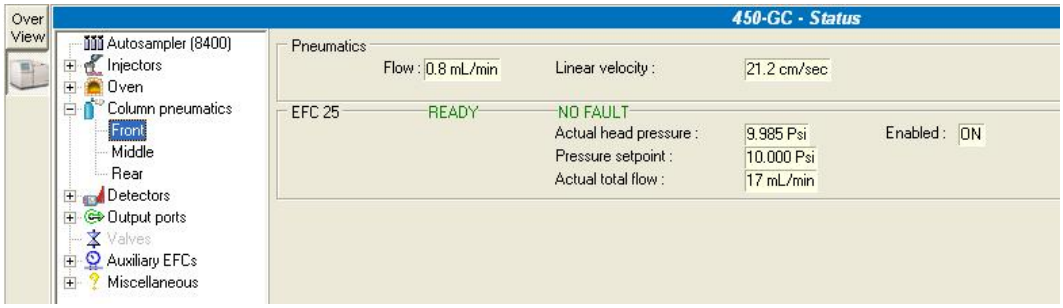
Linear velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual head pressure: Displays the actual column head pressure at the 400 Series GC.

Pressure setpoint: Displays the programmed column head pressure setting in the active method.

Total flow setpoint: Displays, in mL/min, the programmed total flow rate in the active method.

Type 25 EFC Status screen



The status display includes the following parameters:

Ready or *Not Ready*: The Type 25 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 25 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

Fault or *No Fault*: Displays if a fault in the Type 25 EFC component has occurred.

Flow: Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Linear velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual head pressure: Displays the actual column head pressure at the 400 Series GC.

Pressure setpoint: Displays the programmed column head pressure setting in the active method.

Actual total flow: Displays, in mL/min, the total flow rate through the system.

Detectors Window

The detector status screen depends on the installed detector.

The following parameters are available for all the detectors:

The status display includes the following parameters:
-*Ready*, *Not Ready or OFF:* The detector is Ready if the setpoints have been achieved and stabilized. The detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the detector becomes not ready or goes out of tolerance. The detector is OFF if electronics and Heater are turned OFF.

-No fault or Fault to indicate if an error occurs on the GC.

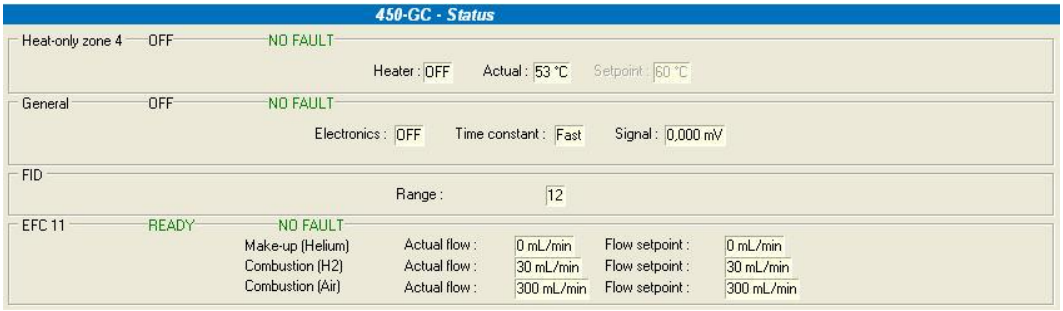
Heater: Displays if the injector oven component is turned OFF or ON at the 400 Series GC.

Actual: Displays the actual temperature of the injector oven at the 400 Series GC.

Setpoint: Displays the injector oven programmed temperature setting in the active method.

Some other parameters are dependent of the type of detector:

FID Status screen



The status display includes the following parameters:
Ready, *Not Ready or OFF* The FID detector is Ready if the setpoints have been achieved and stabilized. The FID detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the FID detector becomes not ready or goes out of tolerance. The FID detector is OFF if electronics and heater are turned OFF.

Fault or *No Fault:* Displays if a fault in the FID detector component has occurred.

Electronics: Displays the FID Electronics setting in the active method.

Time constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual FID detector signal at the 400 Series GC.

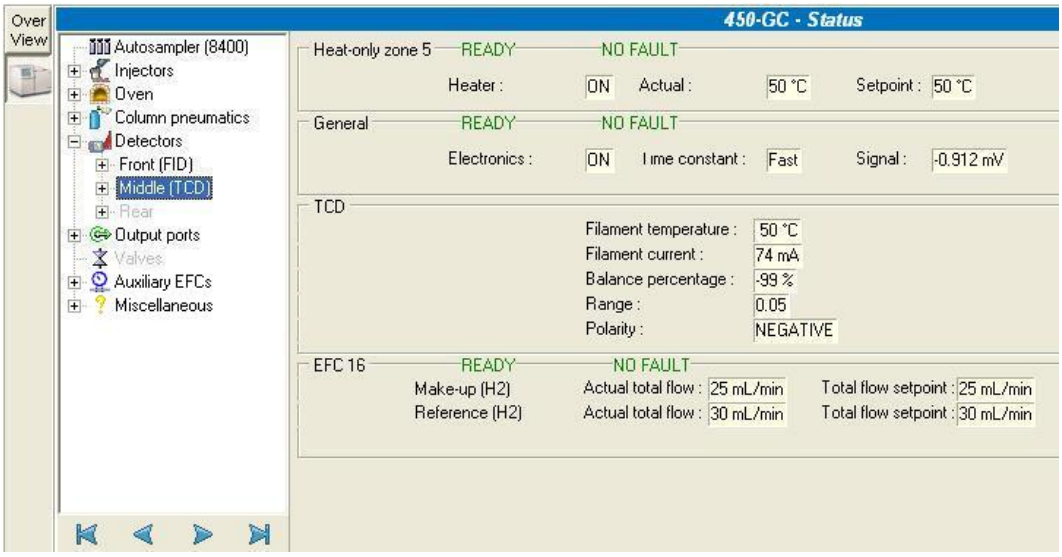
Flame: On or Off.

Range: 9, 10, 11, or 12. Displays the FID Range initial condition setting or the time-programmed setting in the active method.

If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and displays the following parameters:

EFC Type	Parameter	Description
Type 11 EFC	Ready	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

TCD Status screen


Over View
450-GC - Status
Autosampler (8400)
Injectors
Oven
Column pneumatics
Detectors
Front (FID)
Middle (TCD)
Rear
Output ports
Valves
Auxiliary EFCs
Miscellaneous
Heat-only zone 5 READY NO FAULT
Heater : ON Actual : 50 °C Setpoint : 50 °C
General READY NO FAULT
Electronics : ON Time constant : Fast Signal : -0.912 mV
TCD
Filament temperature : 50 °C
Filament current : 74 mA
Balance percentage : -99 %
Range : 0.05
Polarity : NEGATIVE
EFC 16 READY NO FAULT
Make-up (H2) Actual total flow : 25 mL/min Total flow setpoint : 25 mL/min
Reference (H2) Actual total flow : 30 mL/min Total flow setpoint : 30 mL/min

The status display includes the following parameters:

Ready, Not Ready or OFF: The TCD detector is Ready if the setpoints have been achieved and stabilized. The TCD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the TCD detector becomes not ready or goes out of tolerance. The TCD detector is OFF if electronics and heater are turned OFF.

Fault or No Fault: Displays if a fault in the TCD detector component has occurred.

Electronics: Displays the TCD Electronics setting in the active method.

Time constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual TCD detector signal at the 400 Series GC.

Filament temperature: Displays the TCD Filament Temperature setting in the active method.

Filament current: Displays, in mA, the actual TCD current.

Balance percentage: Displays, in %, the TCD bridge balance.

Range: 0.05, 0.5, or 5.0. Displays the current TCD Range.

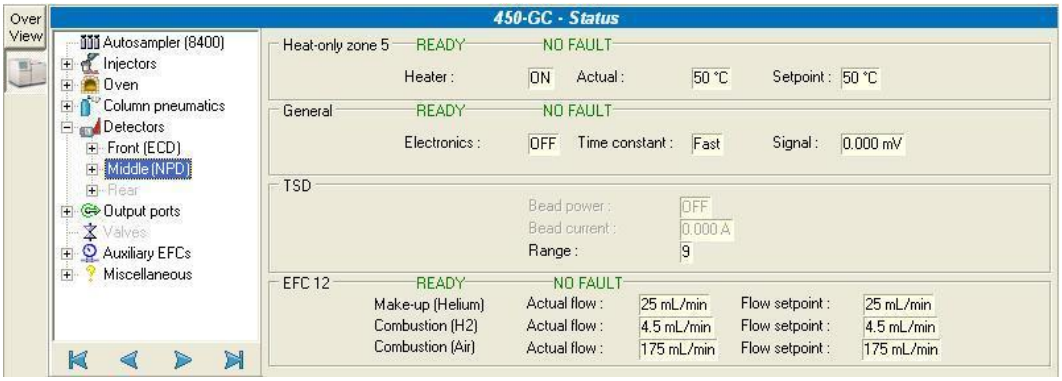
Polarity: Displays the current TCD Polarity.

If the detector Electronic Flow Control module is installed, the Type XY EFC section will appear. Three EFC modules can be used with the TCD detector.

The table below shows the corresponding EFC status items:

EFC Type	Parameter	Description
Type 13 EFC	Ready	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
Type 14 EFC	Ready	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Helium, Nitrogen, or Argon make up.
	Reference	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Helium, Nitrogen, or Argon reference.
Type 16 EFC	Ready	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred.
	Makeup	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Hydrogen make up.
	Reference	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Hydrogen reference.

NPD Status screen



The status display includes the following parameters:

Ready, *Not Ready or OFF*: The NPD detector is Ready if the setpoints have been achieved and stabilized. The NPD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the NPD detector becomes not ready or goes out of tolerance. The NPD detector is OFF if electronics and heater are turned OFF.

Fault or *No Fault*: Displays if a fault in the NPD detector component has occurred.

Electronics: Displays NPD Electronics setting in the active method.

Time constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual NPD detector signal at the 400 Series GC.

Bead power: Displays the current NPD Bead Power.

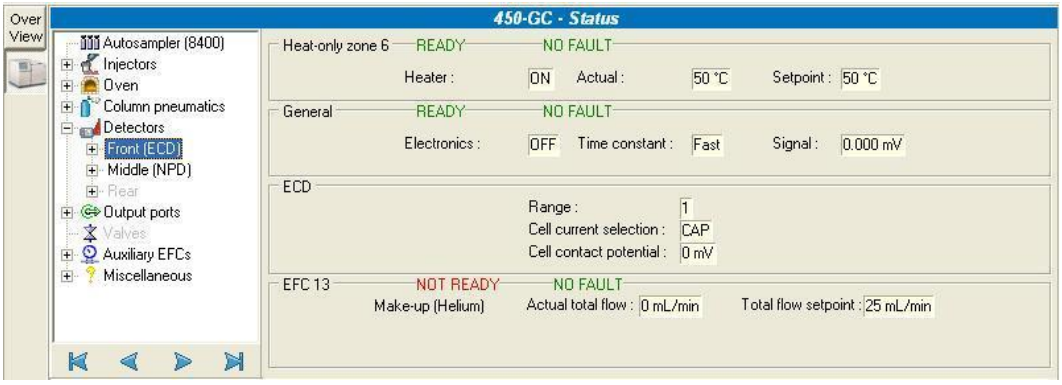
Bead current: Displays the NPD Bead Current setting in the active method.

Range: 9, 10, 11, or 12. Displays the current NPD Range.

If the detector Electronic Flow Control module is installed, the Type 12 EFC section will appear and displays the following parameters:

EFC Type	Parameter	Description
Type 12 EFC	Ready	or Not Ready
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

ECD Status screen



The status display includes the following parameters:
Ready, *Not Ready or OFF*: The ECD detector is Ready if the setpoints have been achieved and stabilized. The ECD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the ECD detector becomes not ready or goes out of tolerance. The ECD detector is OFF if electronics and heater are turned OFF.

Fault or *No Fault*: Displays if a fault in the ECD detector component has occurred.

Electronics: Displays the ECD Electronics setting in the active method.

Time constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

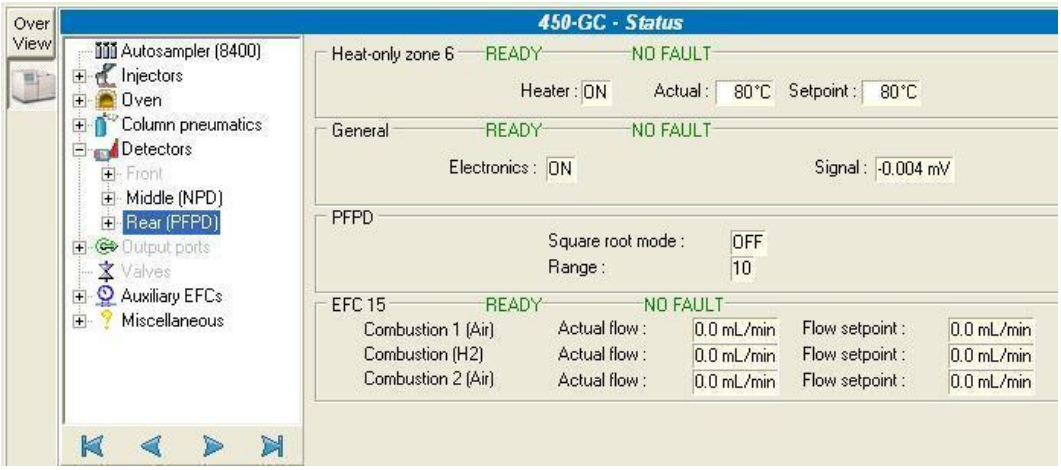
Signal: Displays, in mV, the actual ECD detector signal at the 400 Series GC.

Range: 1 or 10. Displays the current ECD Range.

If the detector Electronic Flow Control module is installed, the Type 13 EFC section will appear and displays the following parameters:

EFC Type	Parameter	Description
Type 13 EFC	Ready	or Not Ready
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate

PFPD Status screen


Over View
450-GC - Status
Autosampler (8400)
Injectors
Oven
Column pneumatics
Detectors
Front
Middle (NPD)
Rear (PFPD)
Output ports
Valves
Auxiliary EFCs
Miscellaneous
Heat-only zone 6 READY NO FAULT
Heater : ON Actual : 80°C Setpoint : 80°C
General READY NO FAULT
Electronics : ON Signal : -0.004 mV
PFPD
Square root mode : OFF
Range : 10
EFC 15 READY NO FAULT
Combustion 1 (Air) Actual flow : 0.0 mL/min Flow setpoint : 0.0 mL/min
Combustion (H2) Actual flow : 0.0 mL/min Flow setpoint : 0.0 mL/min
Combustion 2 (Air) Actual flow : 0.0 mL/min Flow setpoint : 0.0 mL/min

The status display includes the following parameters:
Ready, *Not Ready or OFF*: The PFPD detector is Ready if the setpoints have been achieved and stabilized. The PFPD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the PFPD detector becomes not ready or goes out of tolerance. The PFPD detector is OFF if electronics and heater are turned OFF.

Fault or *No Fault:* Displays if a fault in the PFPD detector component has occurred.

Electronics: Displays the PFPD Electronics setting in the active method.

Signal: Displays, in mV, the actual PFPD detector signal at the 400 Series GC.

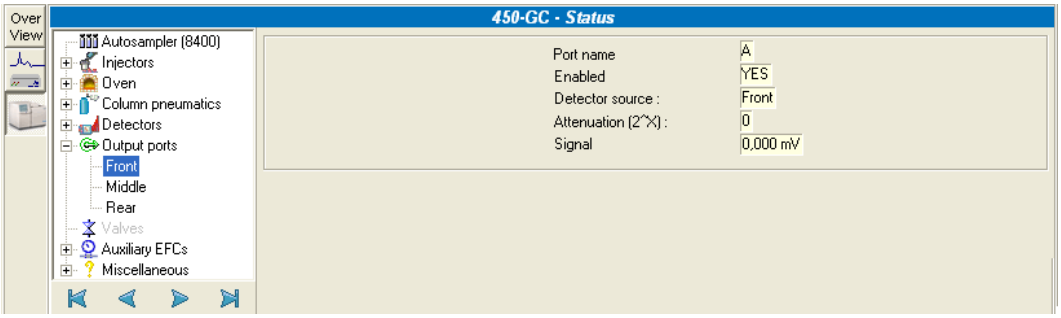
Square root mode: Displays the PFPD Square Root Mode setting in the active method.

Range: 8, 9 or 10. Displays the current PFPD Range.

If the detector Electronic Flow Control module is installed, the Type 15 EFC section will appear and displays the following parameters:

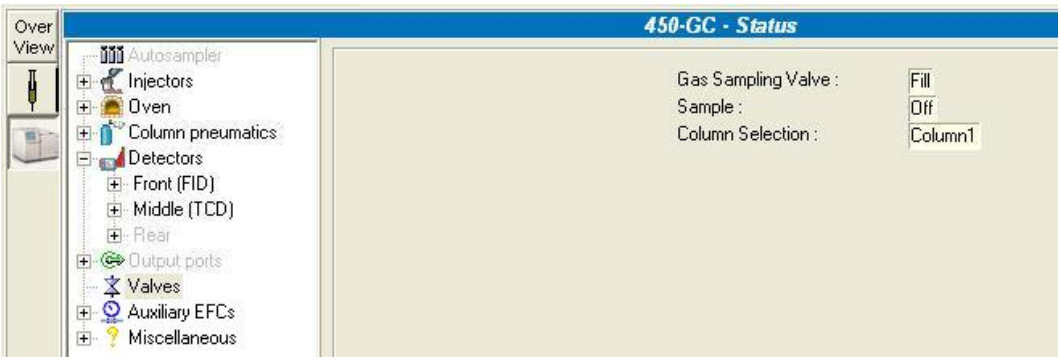
EFC Type	Parameter	Description
Type 15 EFC	Ready	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

Output Ports Window



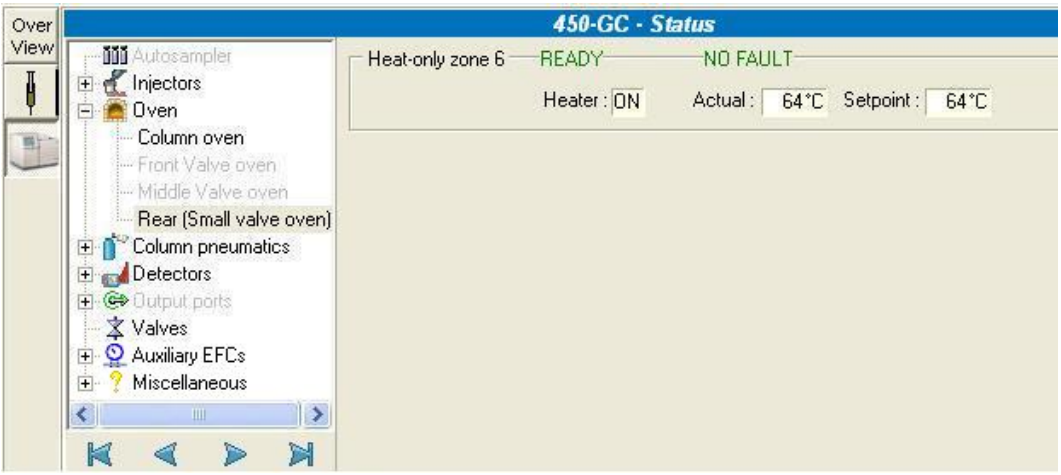
The status screen displays the actual *Detector source*, *Attenuation* and *Signal* for the corresponding port.

Valves Window



If the valves are configured, the status displays the assigned valve name and current state at the 400 Series GC.

If a valve oven is installed, the status displays the following parameters:

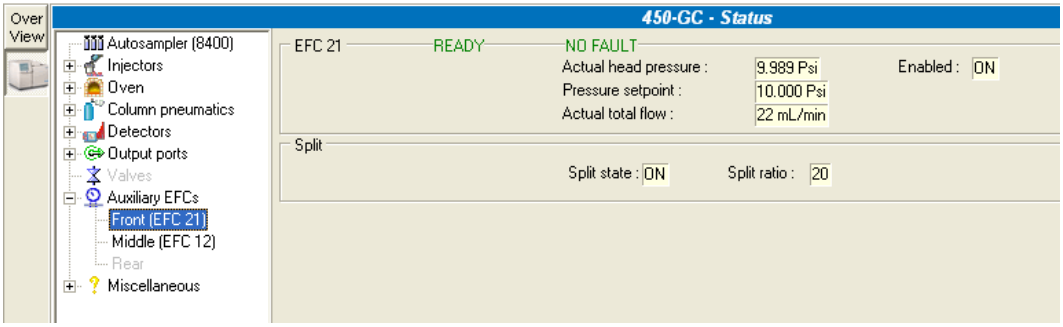


Heater: Displays if the valve oven is turned OFF or ON at the 400 Series GC.

Actual: Displays the actual temperature of the valve oven at the 400 Series GC.

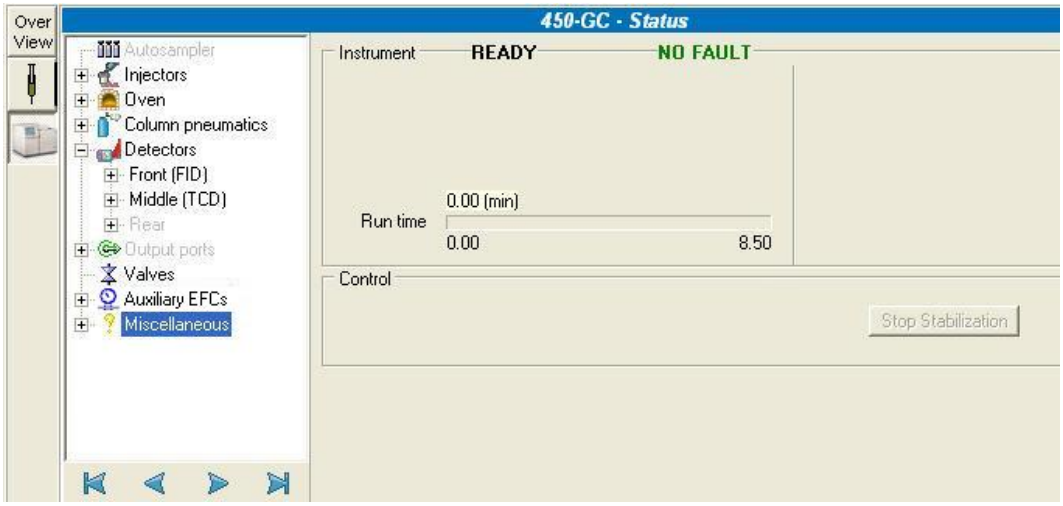
Setpoint: Displays the valve oven temperature setting in the active method.

Auxiliary EFCs Window



For details about the EFC see Column Pneumatics Status and Detectors Status.

Miscellaneous Window



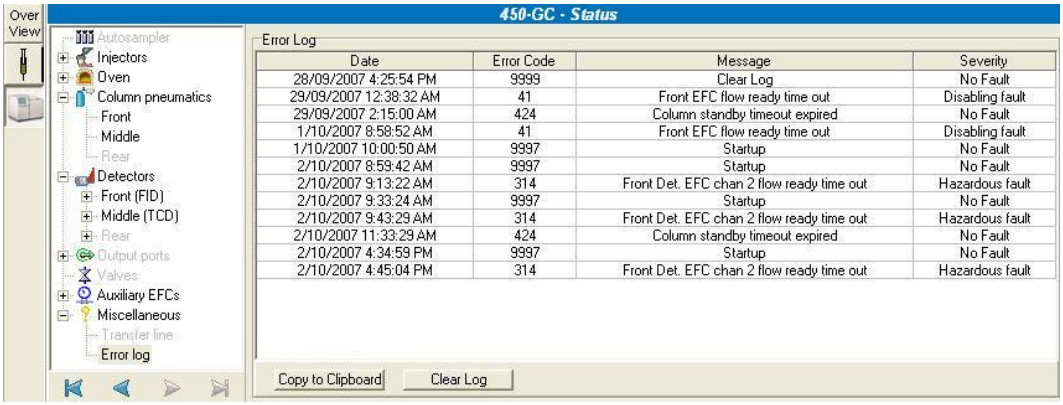
The miscellaneous screen contains general information about the current run and the overall state of the instrument.

The state of the instrument (Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready) is displayed.

A Fault / No Fault indicator is also shown. When a hazardous or disabling fault occurs, any run in progress will halt and the affected component will shut down. If the fault is recoverable, then the run is not terminated.

The run time bar displays the elapsed time in minutes since the beginning of the run and the end time.

Error log Window


450-GC - Status
Over View
Autosampler
Injectors
Oven
Column pneumatics
Front
Middle
Rear
Detectors
Front (FID)
Middle (TCD)
Rear
Output ports
Valves
Auxiliary EFCs
Miscellaneous
Transfer line
Error log
Error Log
Date | Error Code | Message | Severity
28/09/2007 4:25:54 PM | 9999 | Clear Log | No Fault
29/09/2007 12:38:32 AM | 41 | Front EFC flow ready time out | Disabling fault
29/09/2007 2:15:00 AM | 424 | Column standby timeout expired | No Fault
1/10/2007 8:58:52 AM | 41 | Front EFC flow ready time out | Disabling fault
1/10/2007 10:00:50 AM | 9997 | Startup | No Fault
2/10/2007 8:59:42 AM | 9997 | Startup | No Fault
2/10/2007 9:13:22 AM | 314 | Front Det. EFC chan 2 flow ready time out | Hazardous fault
2/10/2007 9:33:24 AM | 9997 | Startup | No Fault
2/10/2007 9:43:29 AM | 314 | Front Det. EFC chan 2 flow ready time out | Hazardous fault
2/10/2007 11:33:29 AM | 424 | Column standby timeout expired | No Fault
2/10/2007 4:34:59 PM | 9997 | Startup | No Fault
2/10/2007 4:45:04 PM | 314 | Front Det. EFC chan 2 flow ready time out | Hazardous fault
Copy to Clipboard
Clear Log

The Error log screen contains error logs from the instrument.

Press the Clear Log button to reset the GC error logs

Press the Copy to Clipboard button to copy all error logs and have the possibility to paste it in a text editor file.

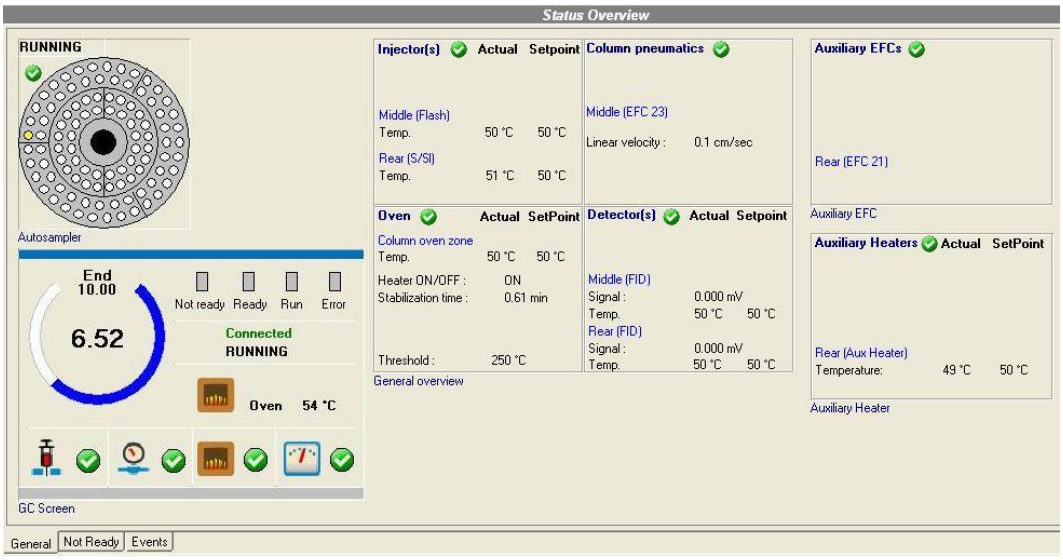
NOTE: When an error occurs on the GC a pop-up window warns you of the instrument error, stop the acquisition and the sequence and add a line in this error logs screen.

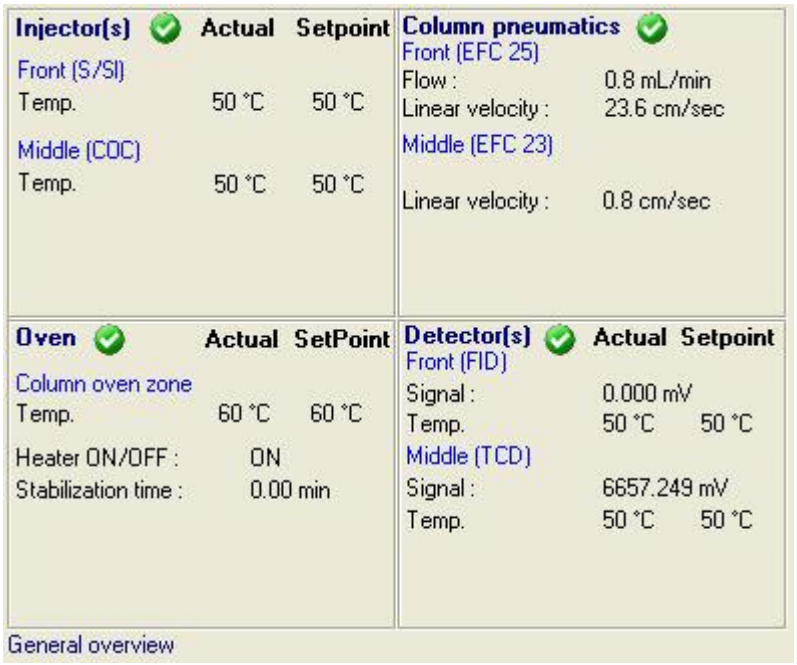
Overview Window

Click on the Over View button: the ***Status Overview*** window is displayed and contains three tabs (to configure this screen see the chapter "*Configuring the synopsis*"):

General Tab*:* displays the synopsis of the GC, where some current values can be read (temperatures, pressures, signal, etc.), for all GC modules.

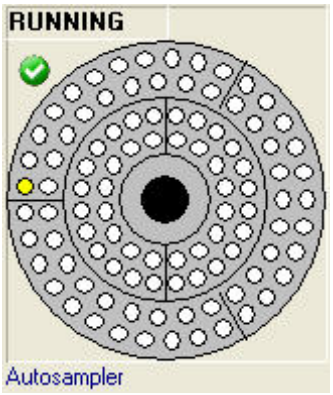
The general overview





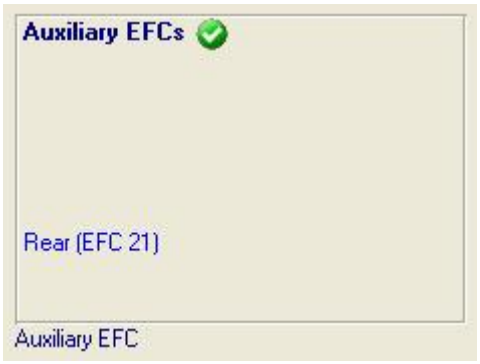
The general overview displays the state of the modules (Injectors, Column pneumatics, Oven, Detectors), the flow and temperature (current and setpoint) and the signal value.

The Autosampler



In the Autosampler module, when the mouse points to a colored vial (yellow for current vial, green for already used vial, and red for missing vial), the current vial number and the number of injections are displayed.

The Aux EFCs screen:



This screen is only visible if Aux EFCs are available in the configuration of the Instrument.

The Aux Heaters screen:

This screen is only visible if Aux heaters and/or small/Large valve ovens are available in the configuration of the Instrument.

The GC screen:

The GC screen overview displays the sate the modules, without temperature, pressure, etc. values.

The colored circles indicate the state of the GC.

: The Green circle means READY

: The Yellow circle means NOT READY

: The Grey circle means OFF

: The Red circle means ERROR

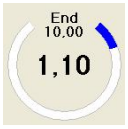
The general GC state (Not ready, Ready, Run, Error):

LEDs are lighting or climbing as on the GC.

The GC connection state: connected or not connected:

The GC state or analysis phase: Ready, Equilibrating, Stabilizing, Pre-Run, Sample Prep, Running, Fault: For example:

The GC oven current temperature:

The running acquisition time and the total time: 

Note that during the stabilizing phase, the running time is displayed in Yellow not in Blue. Clicking on the clock displays the remaining time instead of the current acquisition time.

Not Ready Tab*:* contains the not ready information sent by the GC.

Events Tab: contains the events that have occurred on the instrument.

Varian 430 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501496
Revision D

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the GC Communications 3
    Ethernet Communications 3
  Configuring the Driver 5
    Configuring the 430 GC 5
    Configuring the Synopsis 20
Building a Method 23
  Creating a New Method 23
  Control Method Section for the 430 GC 25
    Autosampler Control 26
    Injector Control 31
    Column Oven Control 32
    Column Pneumatics Control 33
    Detector Control 35
    External Events Control 39
    Miscellaneous Control 40
Starting and Viewing an Acquisition 41
  Quick Start and Sequence 41
    Quick Start (Single Acquisition) 41
    Sequence 42
  Running Acquisition Status 42
    Viewing a Running Acquisition 42
    Status of the 430 GC 42
  430 GC Faults 53
  Autosampler Faults 54

Introduction

This document describes the configuration of the Bruker/Varian 430 GC driver. It also explains how to build a control method for this driver, how to start and view a running acquisition, and what actions are available during an analysis.

The 430 GC has a single 1177 split/splitless or a 1041 injector equipped with Injector Electronic Flow Control, an FID or a TCD detector with Electronic Flow Control, and optionally, a keypad and Ethernet communications.

The CompassCDS Configuration Manager allows you to configure the 430 GC without a keypad for the appropriate column dimensions and temperature limits, and to perform EFC and autosampler calibrations. All these functions can be accomplished locally when the 430 GC is equipped with a keypad.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

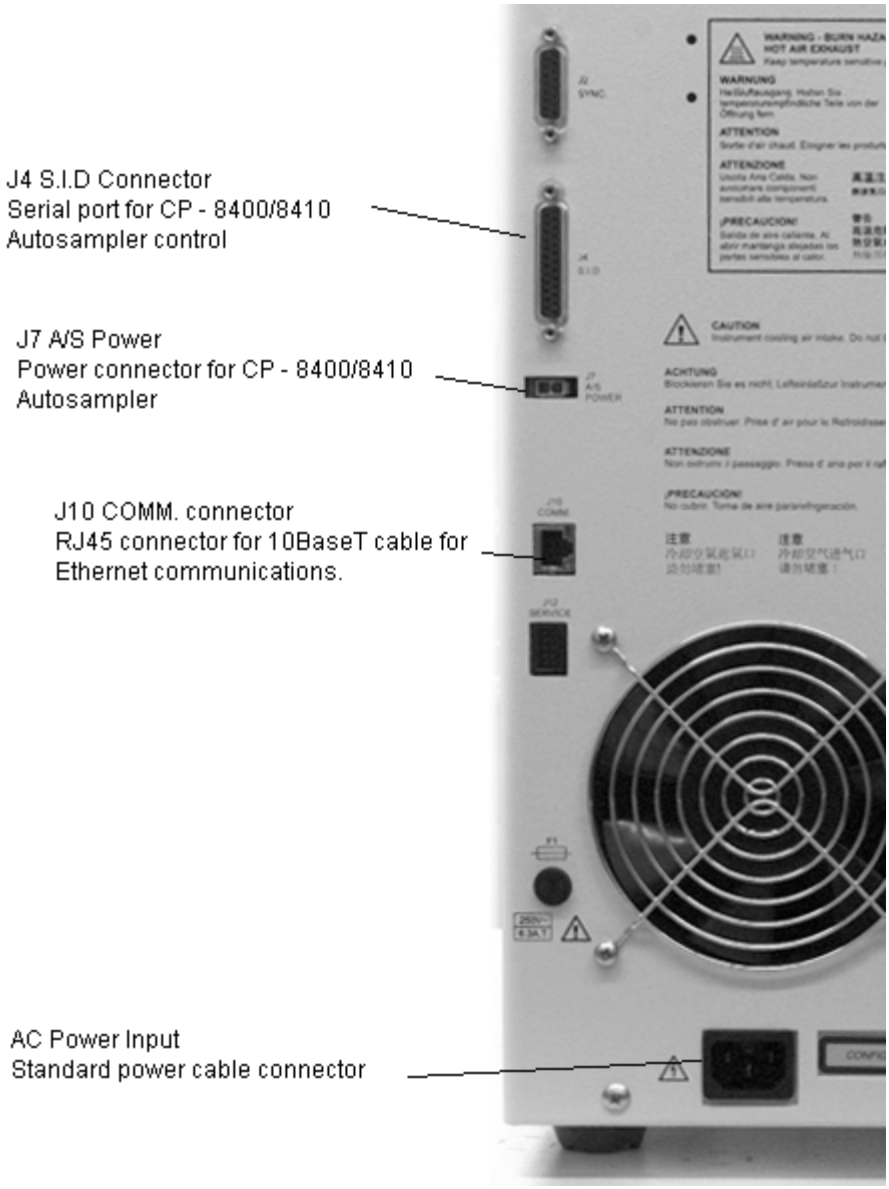
Configuring the GC Communications

Ethernet Communications

The 430 Gas Chromatograph uses Ethernet® as the method of communications for instrument control and for sending digital data to the external data system.

The Ethernet connection is made at the back at the 430 GC (J10 COMM. connector). There are two types of Ethernet cables:

- An Ethernet crossover cable is used when the 430 GC is connected directly to the CompassCDS workstation PC and the PC is not connected to a company network.
- A standard Ethernet patch cable is used when the 430 GC is connected to a company Ethernet network. In this case, you will need to use an Ethernet 10BaseT hub or switch.



The 430 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server is used to send IP addresses to TCP/IP devices.

The BOOTP Server lists Ethernet (MAC) addresses along with the IP addresses that are to be assigned to the corresponding devices.

To know how to configure the BOOTP server, refer to the CompassCDS installation Guide.

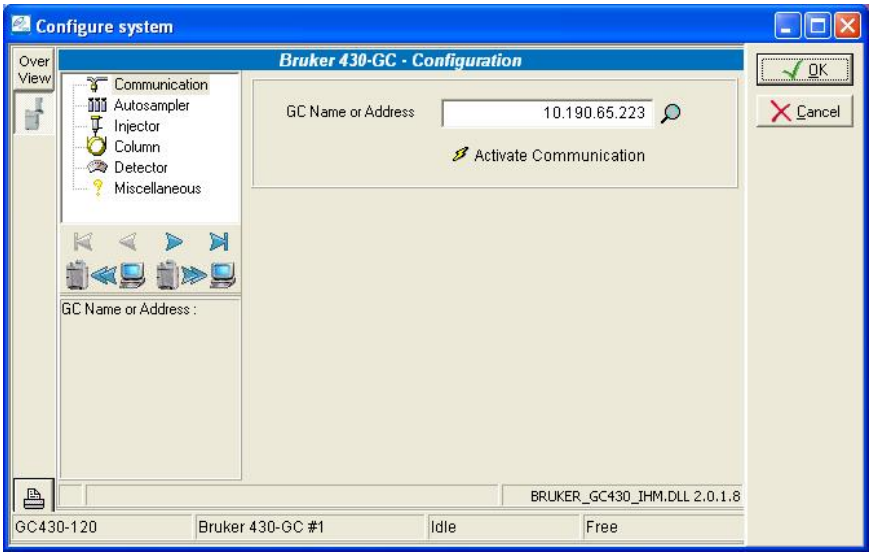
NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the 430 GC

Click on the button corresponding to the 430 GC driver and the GC configuration screens appear:



The toolbar allows you to easily scroll through the configuration windows:

to select the first configuration window.

to select the previous configuration window.

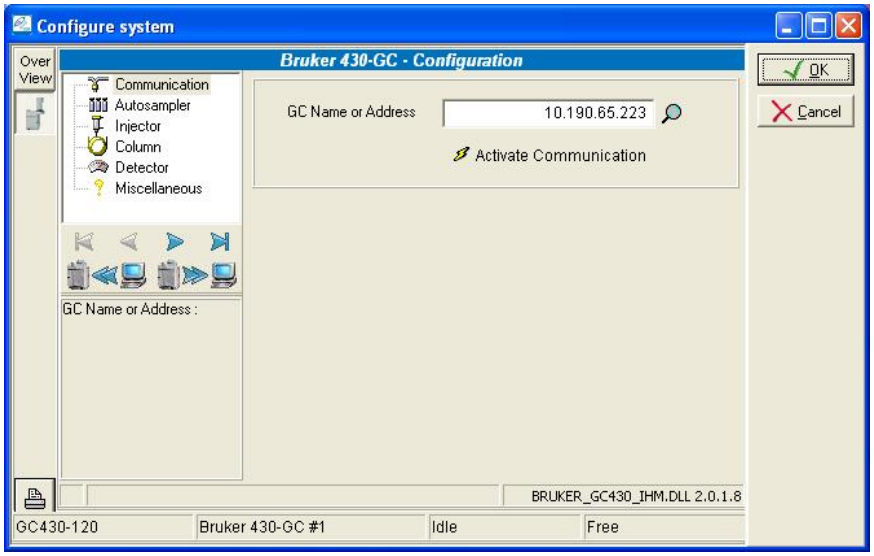
to select the next configuration window.

to select the final configuration window.

to send the configuration to the instrument.

to get the configuration from the instrument.

Communication Window

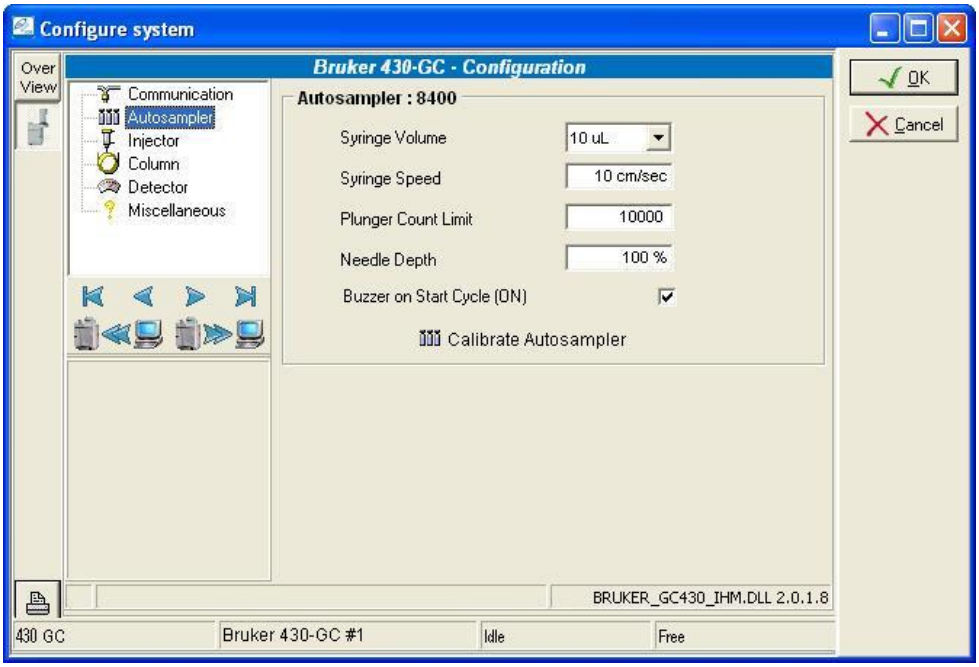


Enter the IP address of the 430 GC (declared in the BOOTP Server) in the GC Name or Address field or click on the button to find the instrument previously declared with the BOOTP Server program and select it.

Press the

button to automatically get the configuration from the instrument.

Autosampler Window



Select from the list the volume (5, 10 or 100 µL) of the syringe you will install. The 430 GC will use this value to set the correct entry selections and any needed internal setting to correctly use the indicated syringe size.

Enter the Syringe Speed (1 to 30 cm/sec, default = 30) in the corresponding field. The injector injection speed parameters define the rate at which the needle will penetrate the injector septum and descend to the set injector needle depth.

Enter the Plunger Count Limit (0 to 100 000, default = 10000): this parameter defines the number of strokes the plunger is expected to survive without significant degradation. Once the entered value is exceeded, a message will be displayed on the GC autosampler status screen, indicating the plunger counter has exceeded the set value.

Enter the Needle Depth (0 to 100%, default = 100) in the corresponding field. This parameter defines how far the needle will penetrate into the designated injector. 100 % causes the needle to be completely inserted to its full 2-inch length.

Check the Buzzer on Start Cycle option to enable the buzzer: a sound will be generated to warn of impending tower movements when this parameter is set to On (default value).

Press the

button to calibrate the autosampler.

NOTE: The autosampler type is automatically detected by the CompassCDS driver.

Autosampler Calibration

If your 430 GC is not equipped with a keypad, the calibration will be performed using the CompassCDS Configuration Manager. The goal of the calibration procedure is to align the autosampler needle with the first vial and with the injector.

NOTE: One basic rule associated with the calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will back up 10 steps when a counterclockwise action is selected but will move one step when a clockwise action is selected.

Vial Calibration

1. To start the vial 0 (or vial 1 if 8410) calibration, make sure a vial with the same form factor and cap as the ones you will be using for your analyses is placed in the 0 position of the carousel (or the vial 1 position for the 8410).

2. Press the

button (or the F1 key) in the Calibrate Vial 0 (or 1) Position field.

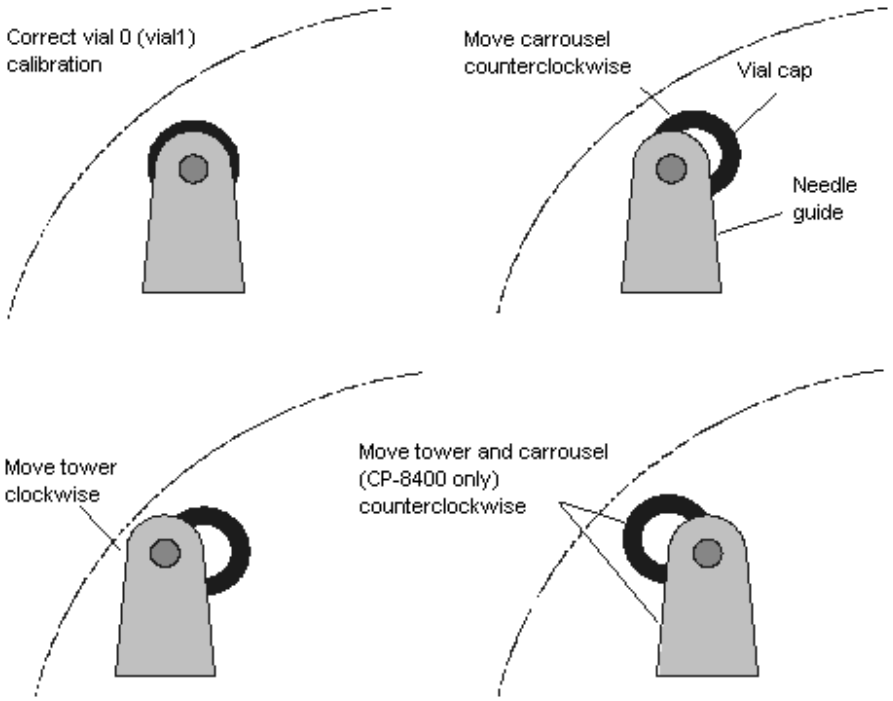
   Calibrating the vial 0 (or vial 1 if 8410) position involves manipulating the positions of three different components. The object of the calibration is to position the needle as closely as possible over the center of the sampling target area of the vial. Upon starting the calibration procedure, the 8400/8410 will rotate the tower, rotate the carousel (on the 8400 only), and lower the syringe sled to the approximate location of vial 0 (or vial 1).

3. After the 8400/8410 has found the approximate vial 0 (or vial 1) position and before going further, visually check that the syringe sled is not resting on the vial top. If it is, use the following buttons, in the Moving Tower / Syringe section, to move the sled so that the needle guide is approximately 1 mm above the vial:

to move the syringe up.

to move the syringe down.

4. Start the calibration process by adjusting the tower position as shown below:



Tower Position Calibration

Use the following buttons, in the Moving Tower / Syringe section, to adjust tower position:

to move the tower 1 step in the clockwise direction each time the button is pressed.

to move the tower 10 steps in the counterclockwise direction each time the button is pressed.

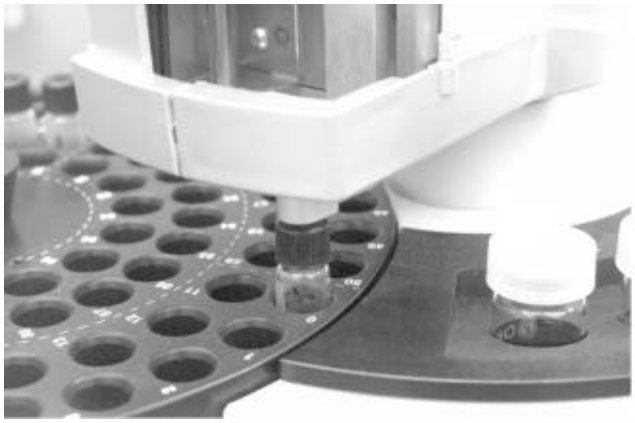
5. Next, for 8400 users only, set the carousel position. Use the following buttons, in the Moving Carousel section, to adjust carousel position:

to move the carousel 1 step in the clockwise direction each time the button is pressed.

to move the carousel 10 steps in the counterclockwise direction each time the button is pressed.

6. Finally, adjust the syringe sled height so that the needle guide is just barely above the vial cap. You should be able to see about a paper's thickness of space between the needle guide and the top of the vial cap. The penetration depth into the vial is measured from the bottom of the needle guide, so this height will give you optimum penetration depth.

   When the Vial 0/Vial 1 calibration is correctly set, the needle guide should be positioned over the vial top as shown below.



Correct Vial Calibration

7. Press the Save Calibration (F2) button (or the F2 key) in the Calibrate Vial 0 (or 1) Position field, to complete the calibration of the vial or press the button to cancel calibration: the autosampler will recover its initial position.

Injector Calibration

After completing the vial position calibration you will need to calibrate the injector position.

1. Press the Start Calibration (F3) button (or the F3 key) in the Calibrate Injector Position field.

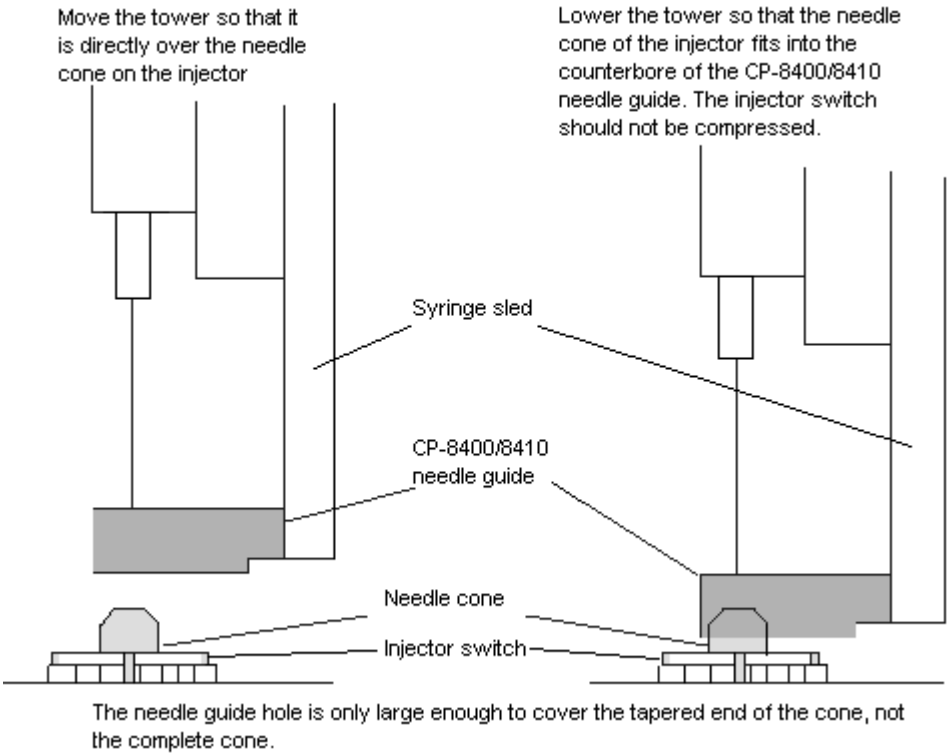
   The syringe tower will rotate so that it is approximately over the injector and the syringe sled will descend to a point near the top of the injector.

   Use the following buttons, in the Moving Tower / Syringe section, to adjust the syringe position:

   to move the syringe up.

   to move the syringe down.

   The needle guide should just cover but not depress the cone on the inject switch as shown below:


Move the tower so that it is directly over the needle cone on the injector
Lower the tower so that the needle cone of the injector fits into the counterbore of the CP-8400/8410 needle guide. The injector switch should not be compressed.
Syringe sled
CP-8400/8410 needle guide
Needle cone
Injector switch
The needle guide hole is only large enough to cover the tapered end of the cone, not the complete cone.

Correct Syringe Sled / Injector Position

2. Move the tower so that it is directly over the needle cone on the injector. Lower the tower so that the needle cone of the injector fits into the counter bore of the 8400/8410 needle guide.

   Use the following buttons, in the Moving Tower / Syringe section, to adjust tower position:

   to move the tower 1 step in the clockwise direction each time the button is pressed.

   to move the tower 10 steps in the counterclockwise direction each time the button is pressed.

NOTE: The injector switch should not be compressed. If the injector switch is compressed, you may experience ‘syringe sled’ errors during autosampler operation. If you are uncertain whether the inject switch is compressing, it is better to raise the syringe sled 1 or 2 steps.

When you have completed the tower and sled movements, the system should look as in the figure below:

Correct Injector Calibration

3. Press the Save Calibration (F4) button (or the F4 key) in the Calibrate Injector Position field, to complete the calibration of the injector or press the button to cancel calibration: the autosampler will recover its initial position.

4. Press the Done button to exit the autosampler calibration screen.

Use of keyboard to adjust positions

The positions of the tower, the syringe or the carousel can also be adjusted by using the following keys:

Tower / Syringe movement

equivalent to the up arrow key.

equivalent to the down arrow key.

equivalent to the left arrow key.

equivalent to the right arrow key.

equivalent to the home key.

Carousel movement

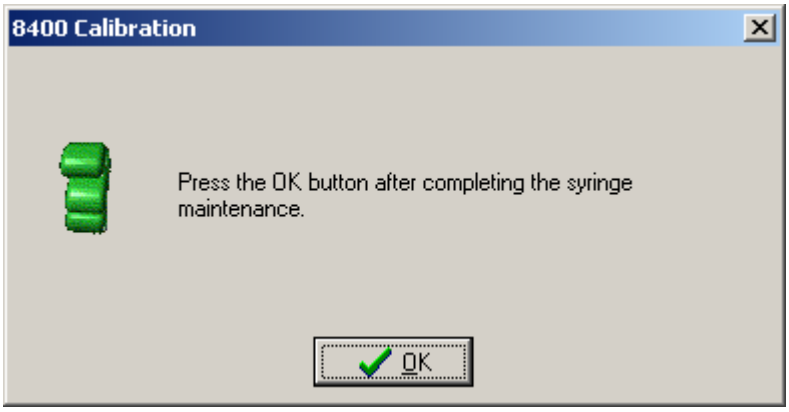
equivalent to the page up key.

equivalent to the page down key.

Syringe Maintenance

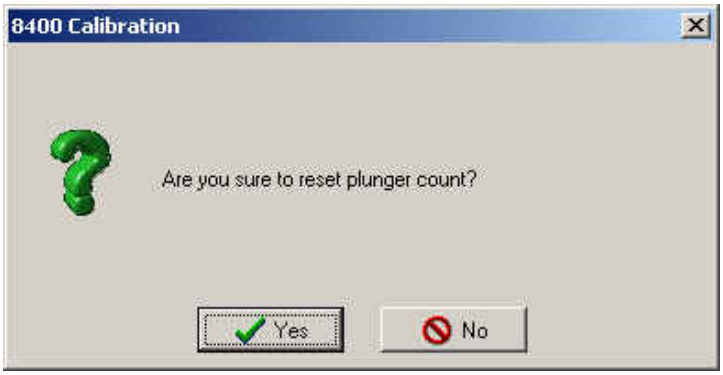
1. Press the Change Syringe (F5) button (or the F5 key): the tower will rotate so as you will have easy access to the syringe (for routine service, syringe removal and replacement…). The buzzer will sound before any tower movement occurs.

2. When the syringe has been changed, press the OK button in the following message screen:



   The tower will return to its previous position and state. The buzzer will sound prior to movement as designated by the Buzzer on Start Cycle setting.

3. Press the Clear Plunger Count (F6) button (or the F6 key) to reset the plunger stroke count to 0. The following warning message appears:



   Validate or cancel the operation by clicking on Yes or No.

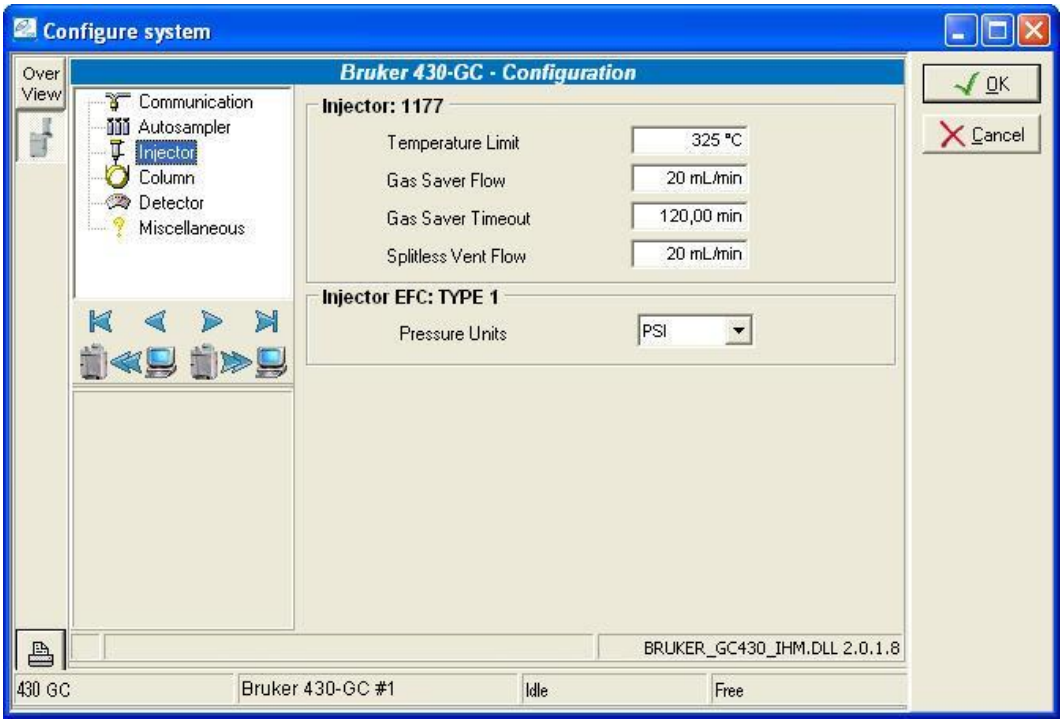
4. Press the Done button to exit the autosampler calibration screen.

Injector Window

1177 Injector

According to the 430 GC model (with or without a keypad), information in this screen is different.

In case of a chromatograph with a keypad, the following screen is displayed:



Injector Parameter Group

Enter the upper temperature limit of the injector in the Temperature Limit field (50 to 450 °C).

Enter the lowest system flow rate that will be maintained during the gas saver period in the Gas Saver Flow field (1 to 100 mL/min, default = 20).

Enter the Gas Saver Timeout in the corresponding field (0 (Off) to 999.99 min). A non-zero value entered for this parameter will cause the system to initiate a timer once a method is activated. If no system actions such as a run start or another method activation occurs before the gas saver timeout is reached, then the system will reduce the flow through the system to the gas saver flow. A method activation action will clear the gas saver flow and bring the system to Ready for subsequent injections.

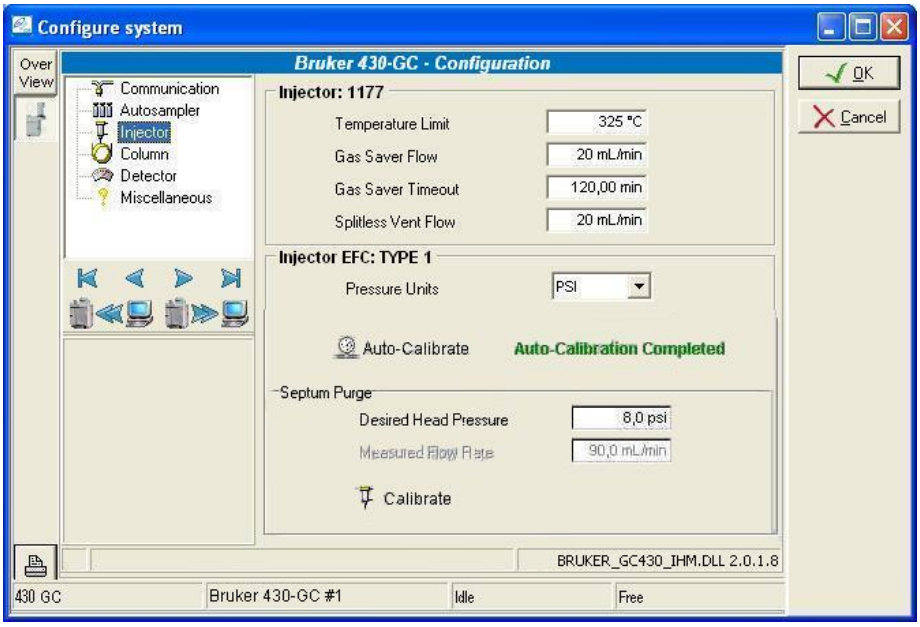
A zero value entered for the gas saver timeout will cause the gas saver flow to be ignored and no gas saver actions will be performed.

Define the Splitless Vent Flow (0 to 500 mL/min) which corresponds to the flow the system will vent when the split valve is left closed for the duration of the run. This flow is diverted before the injector and thus does not influence the splitless nature of the run. This entry is ignored during split and splitless runs in which the split vent is opened.

Injector EFC Type 1 Parameter Group

Select from the list the Pressure Units of the injector EFC (Electronic Flow Control). Three choices are available: PSI, kPa, Bar.

In case of a chromatograph without a keypad, the following screen is displayed:



Parameters are the same that for a chromatograph with a keypad, plus an Auto-Calibrate button and a Septum Purge part.

Click on the Auto-Calibrate button to automatically calibrate the EFC system.

When it is finished, a successful completion or detected problem message is displayed.

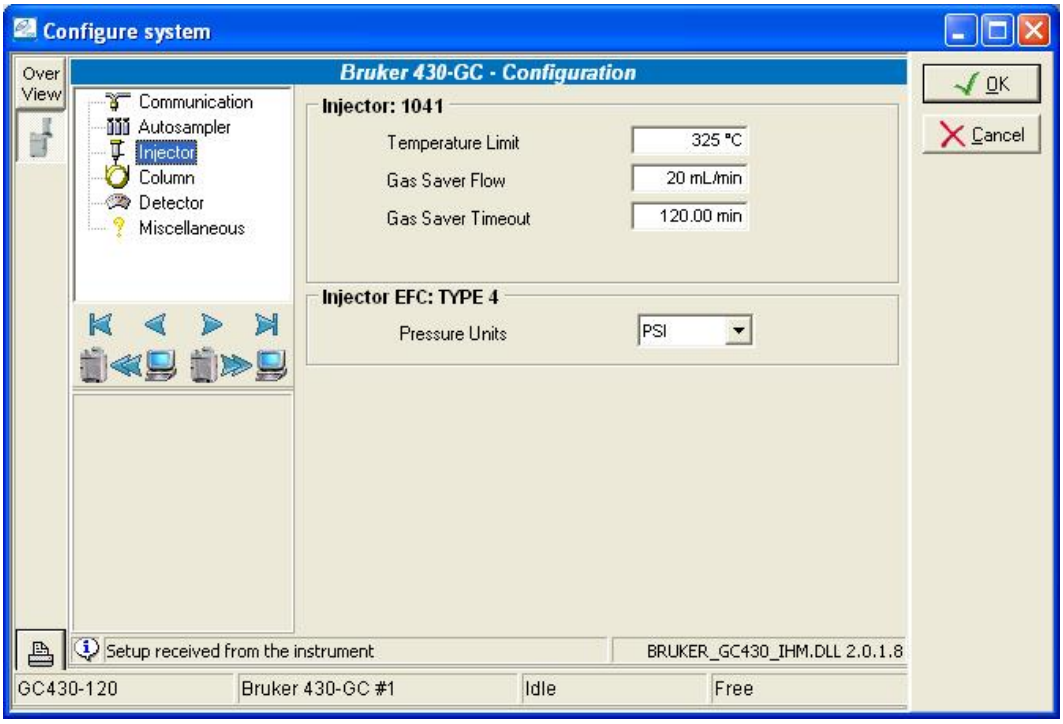
No other GC functions can be performed during Autocalibration.

To calibrate the Septum Purge flow, perform the following steps:

1. Type the pressure in the Desired Head Pressure field.
2. Click on the Calibrate button.
3. Using a flow meter, measure the septum purge flow rate and type it in the Measured Flow Rate field.
4. Click on the Calibrate button.

NOTE: After installing a new column, the septum purge should be calibrated.
The septum purge flow rate is adjustable but is typically set at 3-5 mL/min.

1041 Injector



Injector Parameter Group

Enter the upper temperature limit of the injector in the Temperature Limit field (50 to 450 °C).

Enter the lowest system flow rate that will be maintained during the gas saver period in the Gas Saver Flow field (1 to 100 mL/min, default = 20).

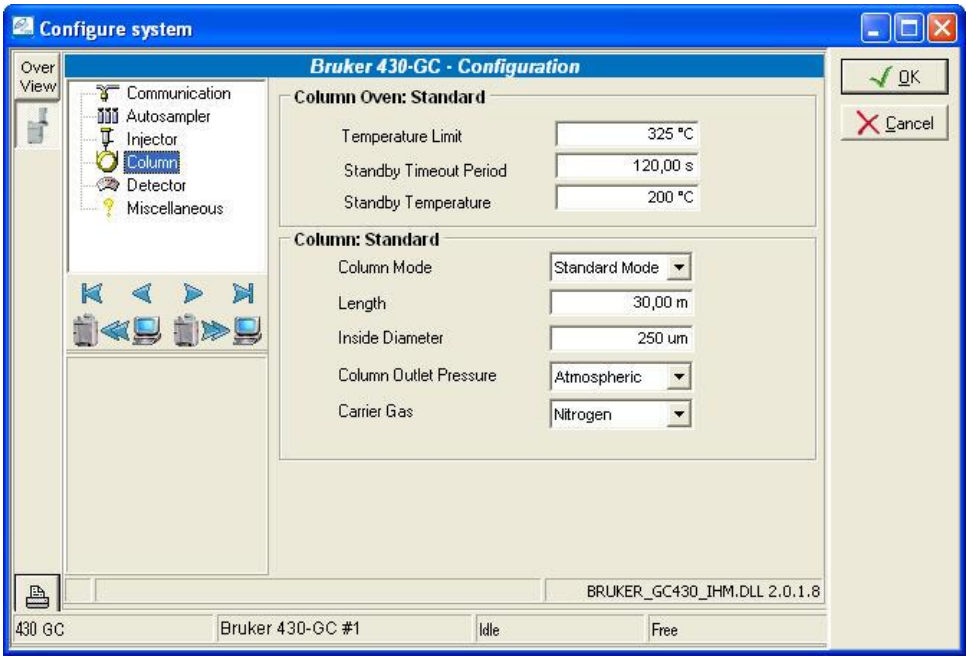
Enter the Gas Saver Timeout in the corresponding field (0 -Off- to 999.99 min). A non-zero value entered for this parameter will cause the system to initiate a timer once a method is activated. If no system actions such as a run start or another method activation occurs before the gas saver timeout is reached, then the system will reduce the flow through the system to the gas saver flow. A method activation action will clear the gas saver flow and bring the system to Ready for subsequent injections.

A zero value entered for the gas saver timeout will cause the gas saver flow to be ignored and no gas saver actions will be performed.

Injector EFC Type 4 Parameter Group

Select from the list the Pressure Units of the injector EFC (Electronic Flow Control). Three choices are available: PSI, kPa, bar.

Column Window



Column Oven Parameter Group

Enter the upper Temperature Limit of the column oven in the corresponding field (50 to 450 °C).

Enter the Standby Timeout Period in the corresponding field (0 to 999 min).

Enter the Standby Temperature in the corresponding field (30 to 250 °C).

When the Column Standby Temperature is enabled, the GC will be held Not Ready until Reset is pressed on the instrument or the Standby Temperature is disabled.

Column Parameter Group:

Select the required Column Mode. Two choices are proposed: Standard Mode (by default) or Rapid MS Mode. Rapid MS Mode is not used with the CompassCDS software at this time.

Enter the column Length (0 to 250 m) and Inside Diameter (0 to 999 µm) in the corresponding fields.

Select from the list the Column Outlet Pressure (Atmospheric or Vacuum – for MS detectors).

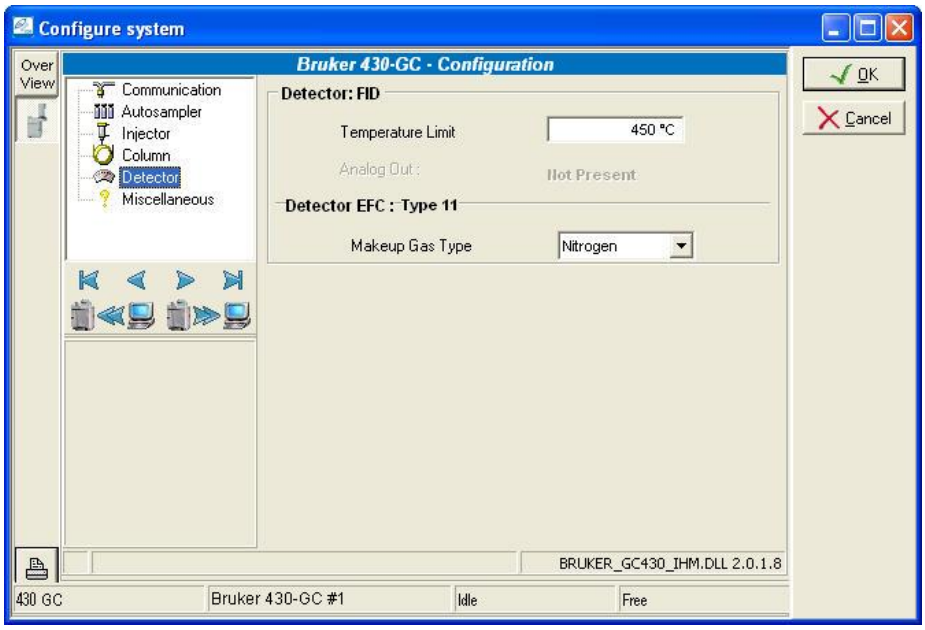
Select the Carrier Gas from the list. The following choices are available: Helium, Hydrogen, and Nitrogen.

Detector Window

FID Detector

Depending on the 430 GC model (with or without a keypad), information on this screen differs:

In the case of a chromatograph with a keypad, the following screen is displayed:



Detector Parameter Group

Enter the upper Temperature Limit of the detector in the corresponding field (50 to 450 °C).

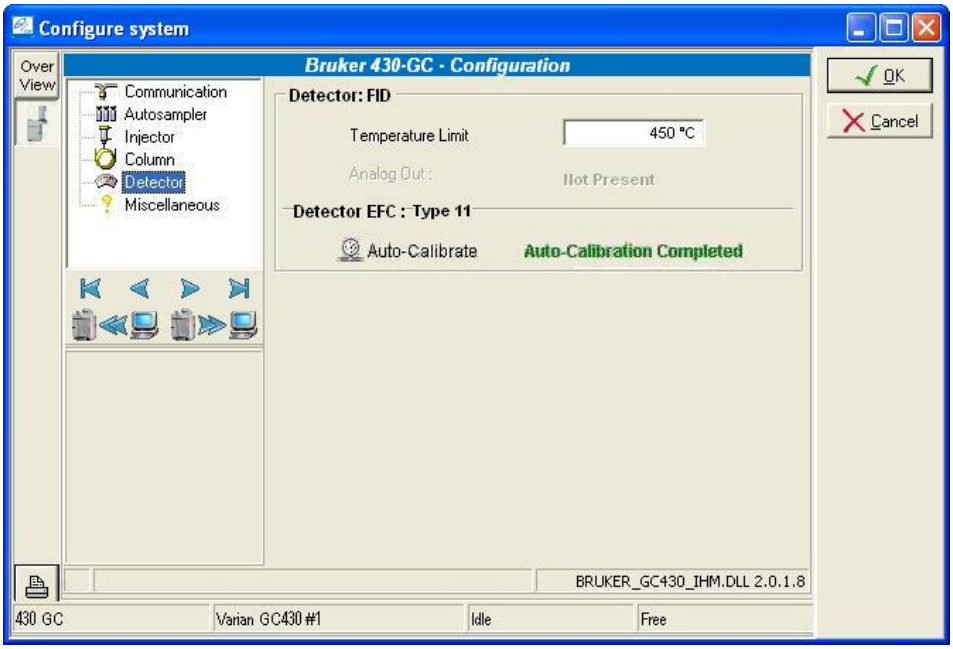
If the Analog Output is configured on the GC, the corresponding field is active and Present is displayed.

Detector EFC Parameter

For FID detectors, the EFC Type 11 is required.

Select the Makeup Gas Type from the list. Three choices are available: Helium, Nitrogen and Argon.

In the case of a chromatograph without a keypad, the following screen is displayed:



Parameters are the same that for a chromatograph with a keypad, plus an Auto-Calibrate button.

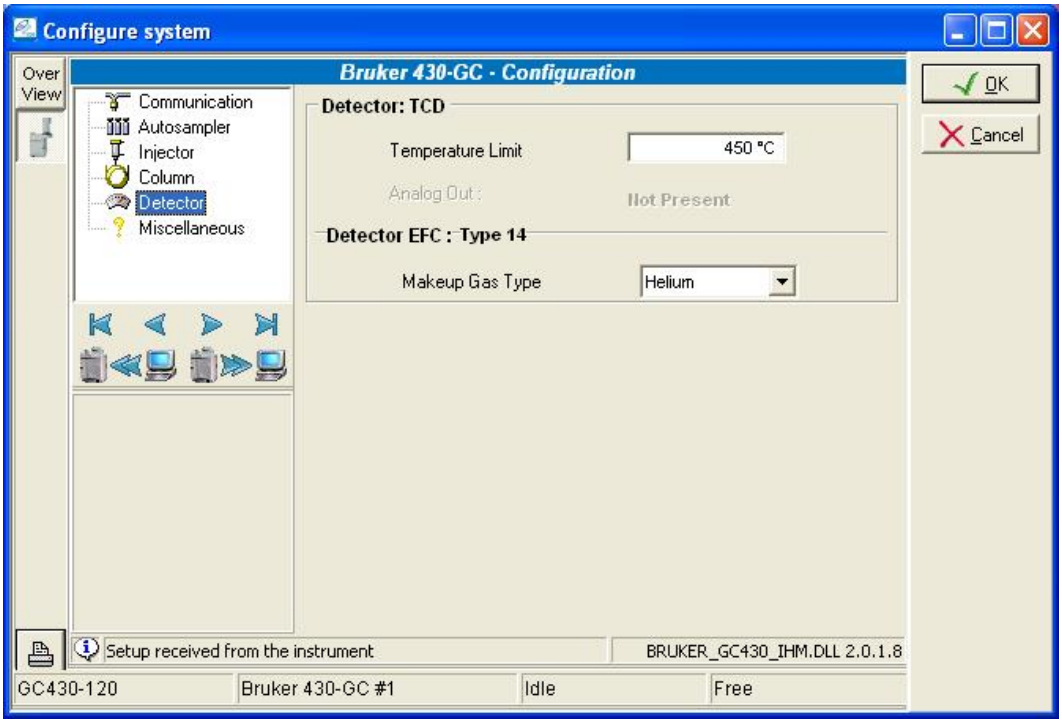
Click on the Auto-Calibrate button to automatically calibrate the EFC system.

When it is finished, a successful completion or detected problem message is displayed.

No other GC functions can be performed during Autocalibration.

NOTE: Autocalibration should be done on a semi-annual basis.

TCD Detector



Detector Parameter Group

Enter the upper Temperature Limit of the detector in the corresponding field (50 to 450 °C).

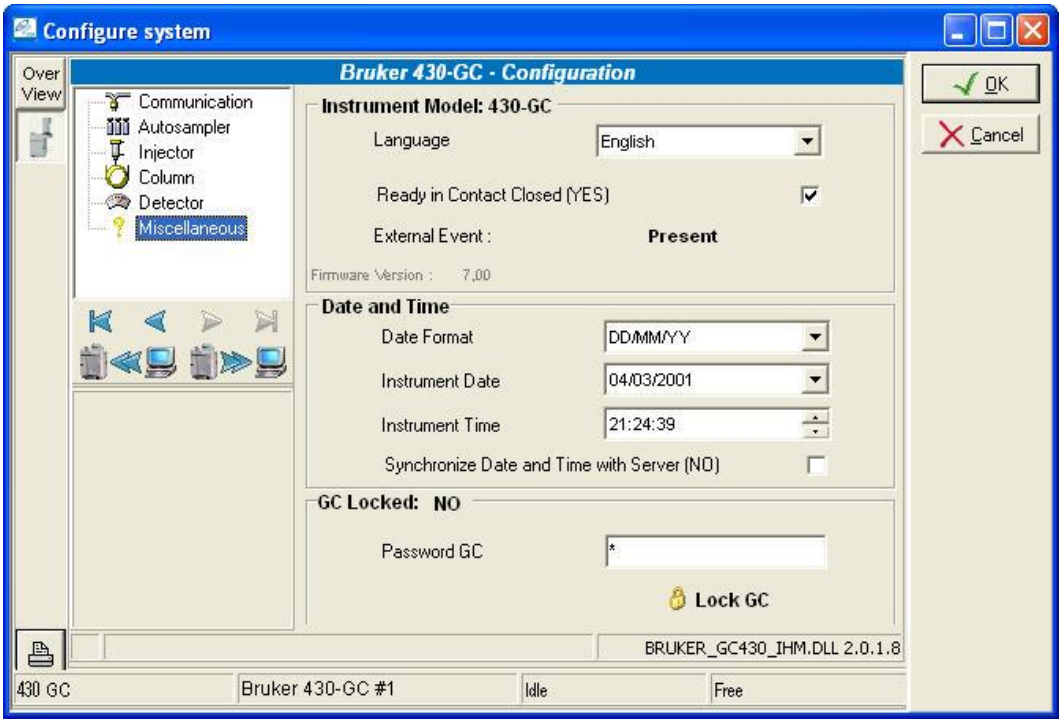
If the Analog Output is configured on the GC, the corresponding field is active and Present is displayed.

Detector EFC Parameter

For TCD detectors, the EFC type 14 is required.

Select the Makeup Gas Type from the list. Three choices are available: Helium, Nitrogen and Argon.

Miscellaneous Window



Instrument Model Parameter Group

Select the Language of the instrument. The available choices include: English, French, Italian, Spanish, German, Katakana (Japanese).

The Ready in Contact Closed option allows you to specify what switch state corresponds to external device Ready. Check the option if the closed state means Ready.

The presence of External Events is also displayed in this screen.

Date and Time Parameter Group

This section allows you to select the Date Format (MM/DD/YY or DD/MM/YY), the Instrument Date and Instrument Time and to choose whether or not to synchronize GC date and time with the server.

GC Locked Parameter Group

To lock or unlock the GC, type the password in the password GC field and press

or

.

If the GC is locked by a password before CompassCDS takes control of the GC, no method can be downloaded into the GC if the password is not specified in the password GC field.

Configuring the Synopsis

In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

1. To save the configuration of these devices, click on the OK button.

2. Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

3. Go back to the System Configuration screen (Properties wizard). A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, then connect these appropriately. To do this, select one anchor from each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

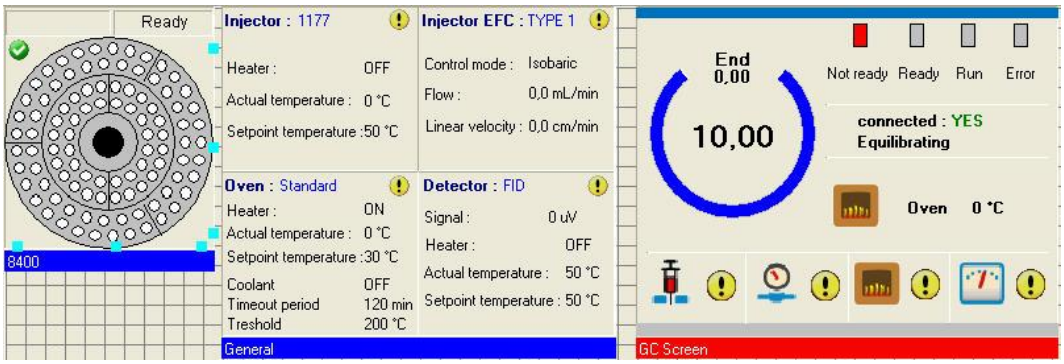
   Click on to delete a selected tube; click on to delete all the tubes.

   Click on to define a background color, or on to make the background transparent.

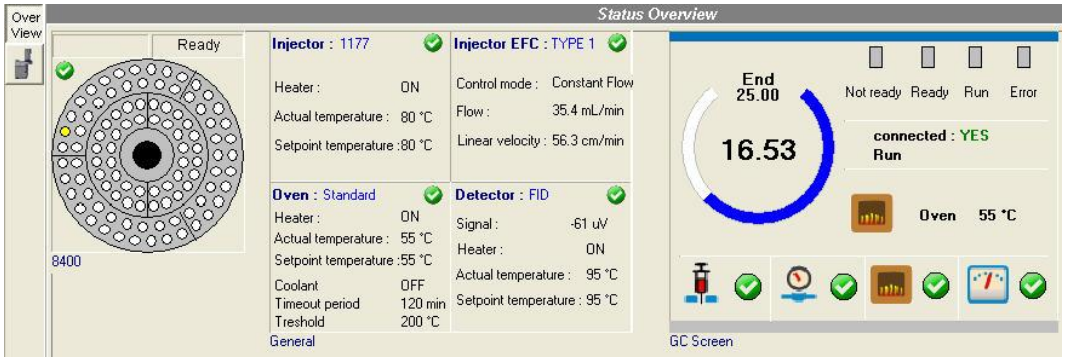
   Click on to change the grid color.

4. Once the synopsis configuration is complete, it will be displayed in the CompassCDS Chromatography Data System, in the Systems tab. In this tab, the Overview will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.), depending on the installed devices.

For example, the following pictures represent the synopsis of the 430 GC:



CompassCDS Configuration Manager Screen



CompassCDS Chromatography Data System Screen

NOTE: Once the system has been created and correctly configured, it must be associated to one or more CompassCDS projects in order to start acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press to print the current 430 GC configuration.

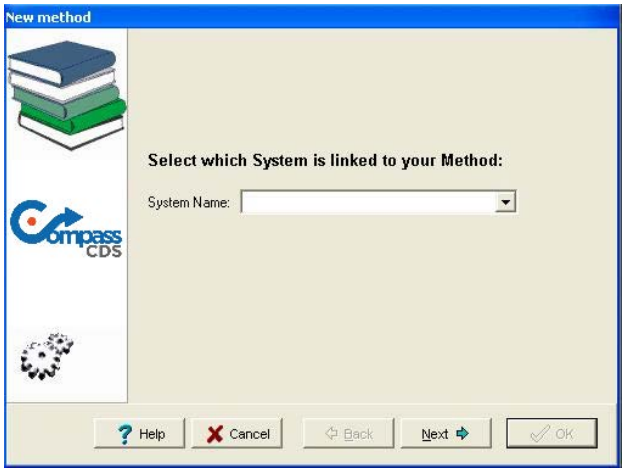
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the method tree sub-sections; however, you must fill in the instrument control and acquisition section prior to starting an acquisition.

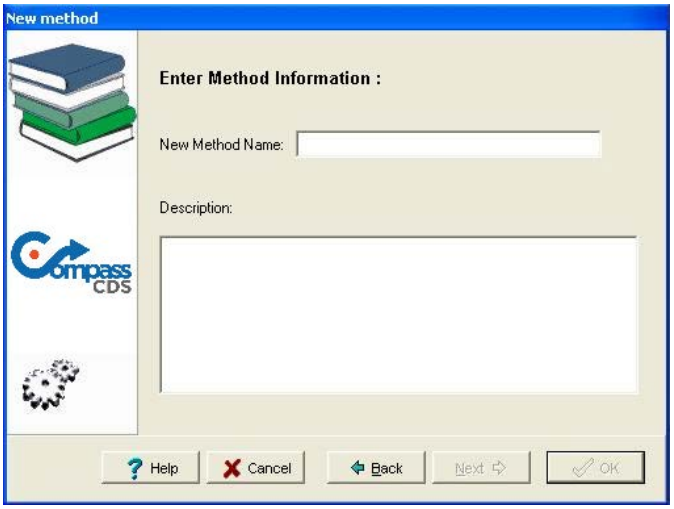
1. To create a new method, select the FILE / NEW METHOD option from the CompassCDS Chromatography Data System main menu.

   A wizard guide will appear and provide assistance during the first steps of method creation:



2. Select the system (chromatograph) to be associated with the method. CompassCDS methods are created for a particular system. When starting an acquisition, you will be prompted for the name of the system and method access is limited to only those methods associated with this system.

3. Once this field is completed, click on the Next button to move to the second step of the method creation:



4. Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

5. Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

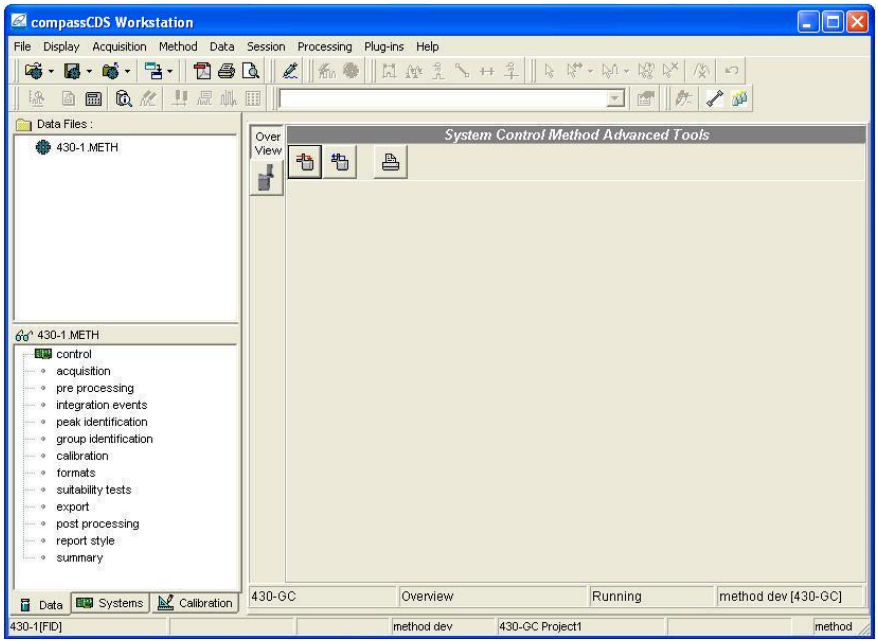
The instrument control and certain parts of the acquisition section must be defined in order to start an acquisition. In the following part of this guide, only the control section of the method for the 430 GC is detailed. Other parameters such as Injection Volume, Vial, and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, refer to the CompassCDS User Guide.

Control Method Section for the 430 GC

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



Press the Over View button to display the System Control Method Advanced Tools window:

to send the current method to the instrument

to get the active method from the instrument

to print the current method

Click on the button to display the 430 GC control method section. It contains seven sub-sections: Autosampler, Injector, Oven, Column Pneumatics, Detector, External Events, and Miscellaneous. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

The toolbar allows you to easily scroll through the control method windows:

to select the first window of the control method.

to select the first window of the control method.

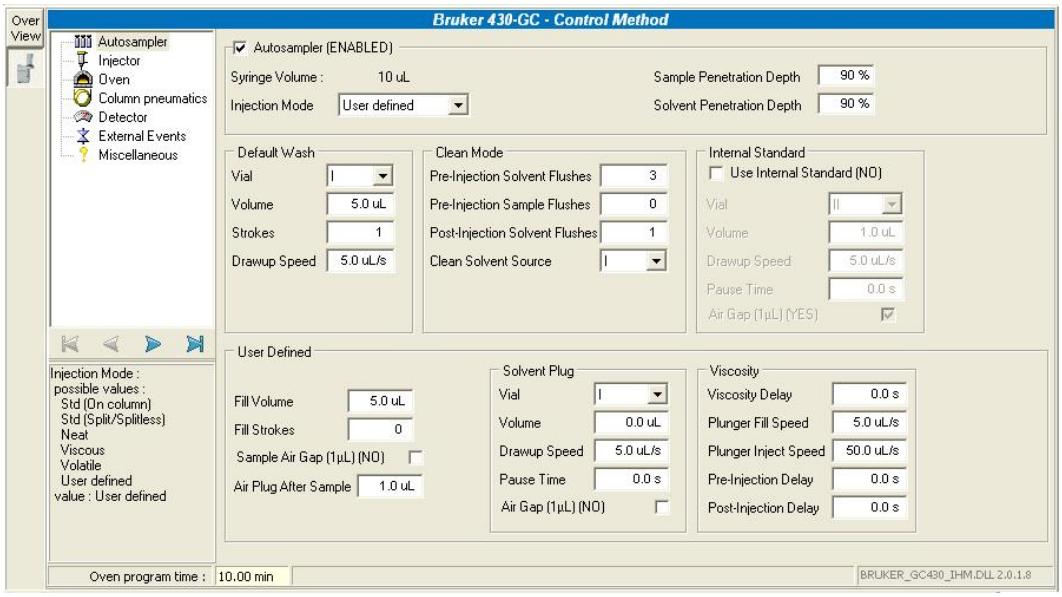
to select the first window of the control method.

to select the final window of the control method.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Autosampler Control

The autosampler window contains sampling parameters for the 8400/8410 Autosampler when attached to the 430 GC:



Autosampler Parameter Group

In this parameter group, define the sampling syringe size (Syringe Volume), the Injection Mode and the Penetration Depth for sample and solvent wash vials.

Parameter	Description
Autosampler	When unchecked, this option allows you to inject manually and to not use the autosampler (when unchecked, all the sampler parameters become non-active).
Syringe Volume (µL)	Selects the size of the syringe that is installed on the instrument.
Injection Mode	Consists of five predefined injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile. A sixth User Defined mode is available and allows you access to all autosampler parameters to fine-tune your injection.
Sample Penetration Depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Penetration Depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.

NOTE:

- The standard mode is the default and typically yields good results in most applications.
- The volatile sampling mode is used for sampling solvents with high vapor pressures at room temperature.
- The neat sampling mode is used for pure samples requiring minimum contamination with wash solvent (this mode does not use a solvent plug).
- The viscous sampling mode is used for samples with a higher viscosity than water.

Default Wash Parameter Group

In the Default Wash fields, define the parameters that will be used during the default cleaning which is used in case automation is stopped or a serious fault is detected.

Parameter	Description
Vial	Specifies which of the three solvent vials will be used by the default cleaning.
Volume (µL)	Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Drawup Speed (µL/s)	Specifies speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

Clean Mode Parameter Group

In the Clean Mode fields, define the pre and post injection syringe clean modes.

Parameter	Description
Pre-Injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample, before injection.
Pre-Injection Sample Flushes	Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.
Post-Injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified), after injection.
Clean Solvent Source	Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.

Internal Standard Parameter Group

The Internal Standard section is displayed when one of the following injection modes is selected: Viscous, Volatile or User-defined.

If the Use Internal Standard option is checked, an internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.

Parameter	Description
Vial	Selects which solvent vial contains the internal standard.
Volume (µL)	Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup Speed (µL/s)	Specifies the speed at which the internal standard will be drawn up into the syringe.

Parameter	Description
Pause Time	Defines how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air Gap	When the option is checked, 1 uL of room air will be drawn into the syringe to create an air gap between the internal standard and the sample

NOTE: When this mode of injection is selected, beware that the total volume (volume of sample injected, entered in the Volume field of the Acquisition method section + Volume of internal standard + volume of any air gaps) does not exceed the maximum syringe volume or the autosampler will be faulted and the GC will stay in the Waiting for injection state.

User Defined Parameter Group

When the User Defined injection mode has been selected, another parameter group is displayed and allows you to define the general, Solvent Plug and Viscosity parameters:

User Defined Parameters:

Parameter	Description
Fill Volume (µL)	Specifies the sample volume that will be used for each fill stroke.
Fill Strokes	Specifies the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.
Sample Air Gap	When the option is checked, 1 uL of room air will be drawn into the syringe to create an air gap before the sample plug.
Air Plug After Sample	Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

Solvent Plug Parameters:

Parameter	Description
Vial	Selects which solvent vial to use for the solvent plug.
Volume (µL)	Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup Speed (µL/s)	Specifies the speed at which the solvent will be drawn up into the syringe.
Pause Time	Defines how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air Gap	When the option is checked, 1 uL of room air will be drawn into the syringe to create an air gap before the solvent plug.

Viscosity Parameters:

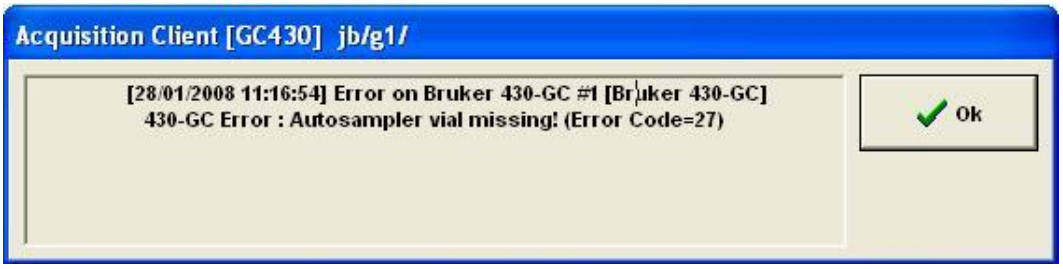
Parameter	Description
Viscosity Delay (sec)	Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Plunger Fill Speed (µL/sec)	Specifies the speed at which the sample will be drawn up into the syringe.
Plunger Inject Speed (µL/sec)	Specifies the speed at which the contents of the syringe will be expelled into the injector.
Pre-Injection Delay (sec)	Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.
Post-Injection Delay (sec)	Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

NOTE: When a vial is missing, the following message appears. You have 10 minutes to replace the sample in the correct vial position before the system skips the missing vial and passes to the next line of the sequence or stops the run. When you have replaced the missing sample, you must go to

k on the instrument icon, select the Miscellaneous tab and click on the button to restart the run.

If you want to skip the missing vial and start the next run, you must press the

button.


Acquisition Client [GC430] jb/g1/
[28/01/2008 11:16:54] Error on Bruker 430-GC #1 [Bruker 430-GC]
430-GC Error : Autosampler vial missing! (Error Code=27)
Ok

Warning message when a vial is missing.

Default Settings for Predefined Autosampler Mode

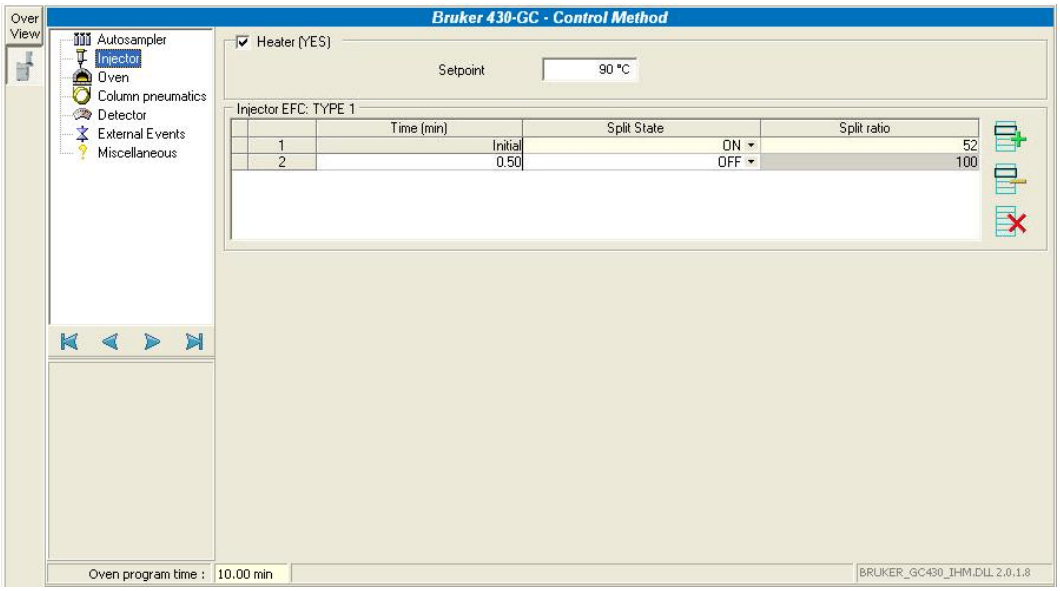
The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

Parameter	Std Split/ Splitless	Std On-Column	Neat*	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, you must use User Defined mode.				
PreDefined Settings:					
Fill Volume	10.0 µL	10.0 µL	10.0	Not used	Not used
Fill Strokes	5	5	6	0	0
Sample Air Gap	No	No	No	No	No
Air Plug after Sample	1.0 µL	1.0 µL	1.0 µL	1.0 µL	1.0 µL
Viscosity Settings:					
Viscosity Delay	0.0 sec	0.0 sec	0.0 sec	6 sec	9.9 sec
Plunger Fill Speed	2.0 µL/sec	2.0 µL/sec	2.0 µL/sec	1.0 µL/sec	1.0 µL/sec
Plunger Inject Speed	50 µL/sec	2 µL/sec	50 µL/sec	1 µL/sec	5 µL/sec
Pre-Injection Delay	0.0 sec	0.0 sec	0.0 sec	0.0 sec	0.0 sec
Post-Injection Delay	0.0 sec	6.0 sec	0.0 sec	0.0 sec	12.0 sec

***Instead of fill strokes, Neat mode fills the syringe with sample at 2 µL/sec then expels it into the waste cup at 50 µL/sec. It does this a total of six times. Then it fills the syringe with sample at 2 µL/sec and expels it back into the sample vial at 50 µL/sec. This "pumping" action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.**

Injector Control

1177 Injector



Check or uncheck the Heater option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the Setpoint field (50 to 450 °C).

Injector EFC Parameter Group

If the injector is connected to a Type 1 EFC, you can build a split ratio time program by using the split event table:

The first row of the spreadsheet contains the Initial Split State and Split Ratio for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed.

The rest of the spreadsheet contains the time-programmed settings for the injector Split Ratio: The Split Valve will be switched to the ratio in each row at the indicated time. If the Split State is ON, then the sample is split according to the Split Ratio specified in the corresponding column. If the state is OFF, the entire sample enters the column.

The split ratio is defined as the column flow plus the split flow, divided by the column flow.

NOTE:

- You must have already configured the Type 1 EFC in the configuration manager (CompassCDS Configuration Manager) before you can program the split ratio.

- You can use a split ratio of 100 after injection to vent the injector of any residual solvent.

- Use a very low split ratio after flushing to conserve carrier gas.

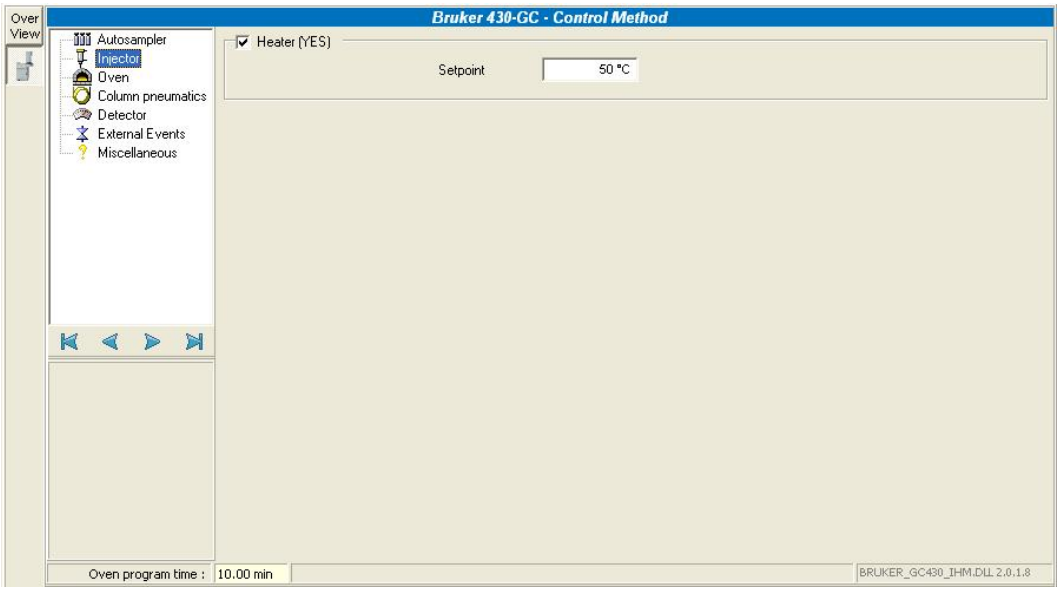
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

1041 Injector

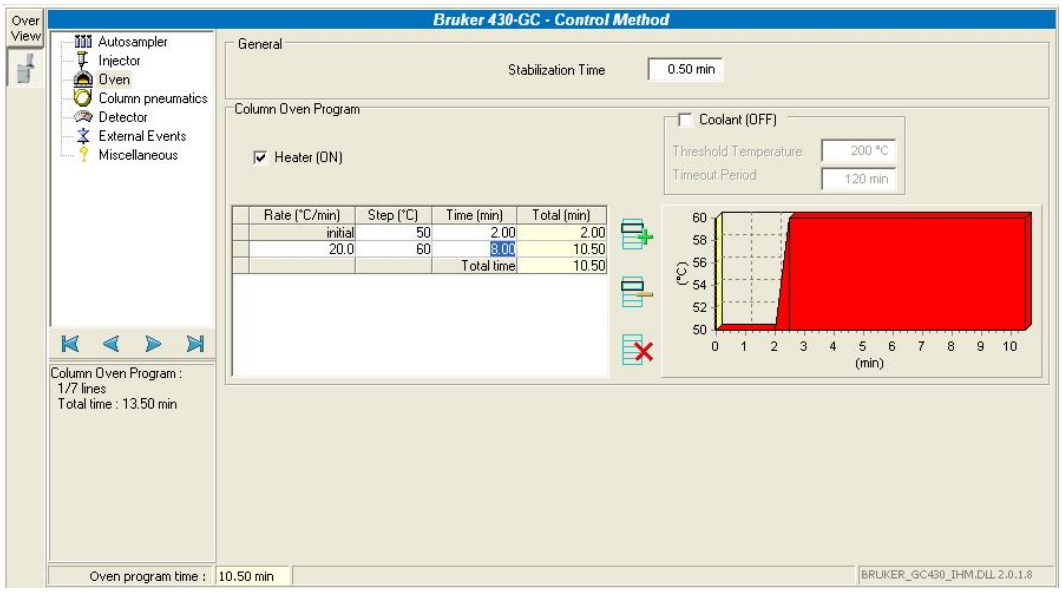


Check or uncheck the Heater option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the Setpoint field (50 to 450 °C).

Column Oven Control

The Column oven window contains the column oven program:



General Parameter

Enter the Stabilization Time in the corresponding field (0.00 to 10.00 min).

Column Oven Program Parameter Group

Check or uncheck the Heater option to turn it ON or OFF.

Use the spreadsheet to build a temperature ramp program to heat and/or cool the column oven.

The first row of the spreadsheet contains the Initial temperature and hold time for the column oven. The column oven will equilibrate to this setting and stabilize for the specified Stabilization Time (defined in the General field), when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the Step column (30 to 450 °C), the Rate (0.1 to 100.0 °C/min) and the Time (0.00 to 999.99 min) the column oven is held at this temperature in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

The graph shows the column oven temperature program.

Check the Coolant option if you want to turn the column coolant valve ON. Specify the temperature for the coolant valve to turn on in the Threshold Temperature field (50 to 250 °C) and the Timeout Period (0 to 999 min).

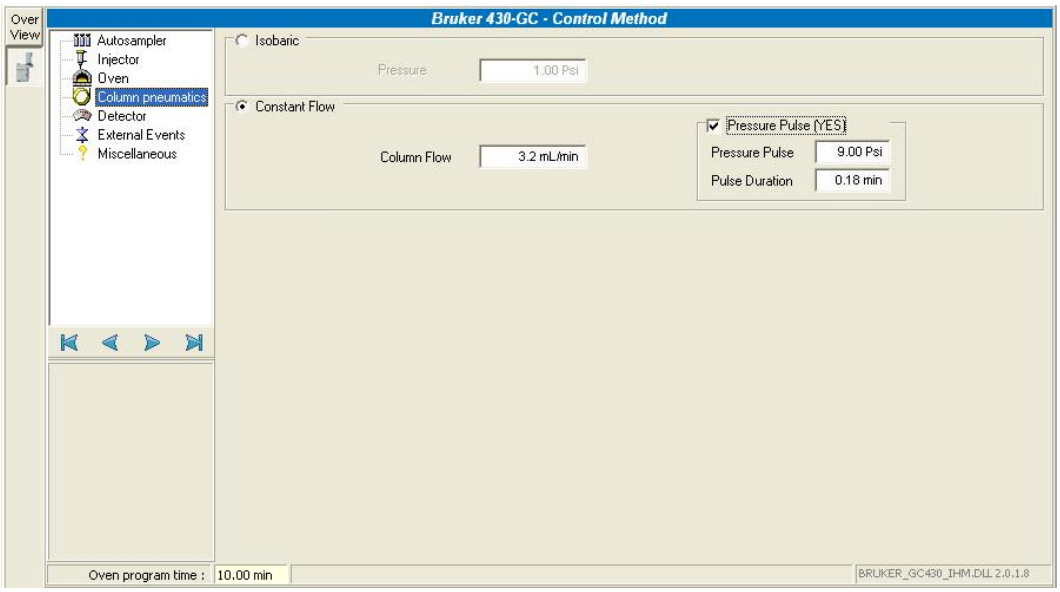
This parameter provides a safety measure to save coolant after the specified time if the column oven fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the timeout period is reached and no further coolant will be applied.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Column Pneumatics Control

The Column pneumatics window contains the Electronic Flow Control (EFC) Program which allows you to specify the pressure ramp of the Type 1 EFC or the pressure ramp and total flow time program of the Type 4 EFC. Type 1 EFC is specially used for the 1177 injector while Type 4 EFC is used for the 1041 injector.

Type 1 EFC



Isobaric Parameter Group

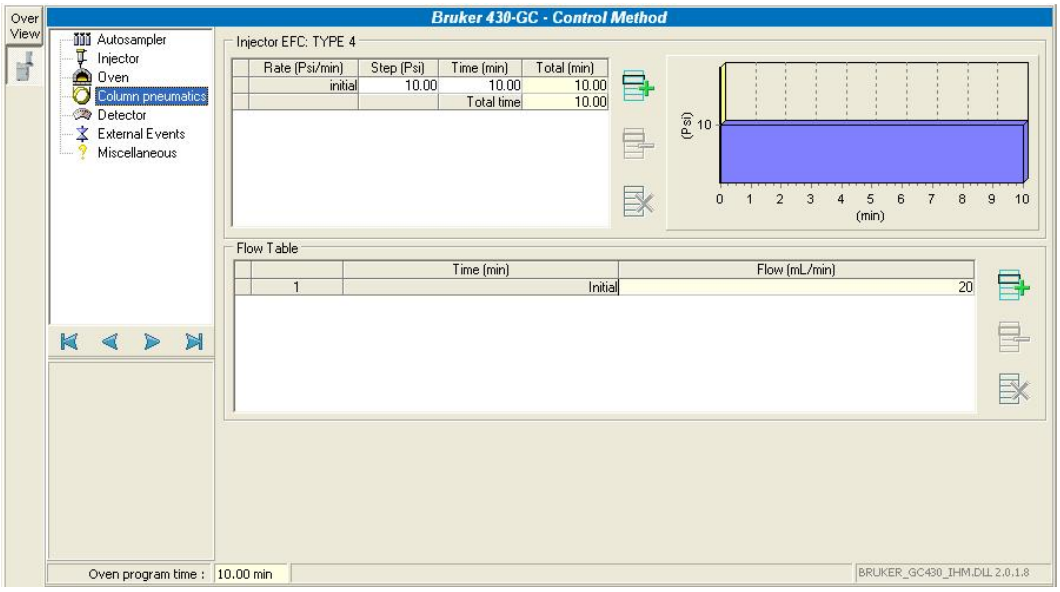
Check the Isobaric option to define a desired gas Pressure in the corresponding field.

Constant Flow Parameter Group

Check the Constant Flow option to disable the isobaric option and enter the desired constant Column Flow in the corresponding field.

Check the Pressure Pulse option to perform a pressure pulse injection. Prior to injection, the column head pressure will change to the Pressure Pulse pressure. After injection, the Pressure Pulse pressure will be maintained for the Pulse Duration.

Type 4 EFC



Injector EFC Parameter Group

Use the first spreadsheet to build a pressure ramp program.

The first row of the spreadsheet contains the Initial pressure and hold time for the Type 4 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the Step column (0.10 to 400.00 PSI), the Rate (0.01 to 400.00 PSI/min) and the Time (0.00 to 999.99 min) the EFC is held at this pressure in the corresponding columns.

NOTE: The graph shows the pressure ramp program.

Flow Table Parameter Group

Use the second spreadsheet to build a flow time program to control the Type 4 EFC total flow.

The first row of the flow spreadsheet contains the Initial Total Flow for the Type 4 EFC.

The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the time-programmed settings for the total flow. The total Flow (1 to 1000 mL/min) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min).

Use the following buttons to edit the table :

to add a line to the table.

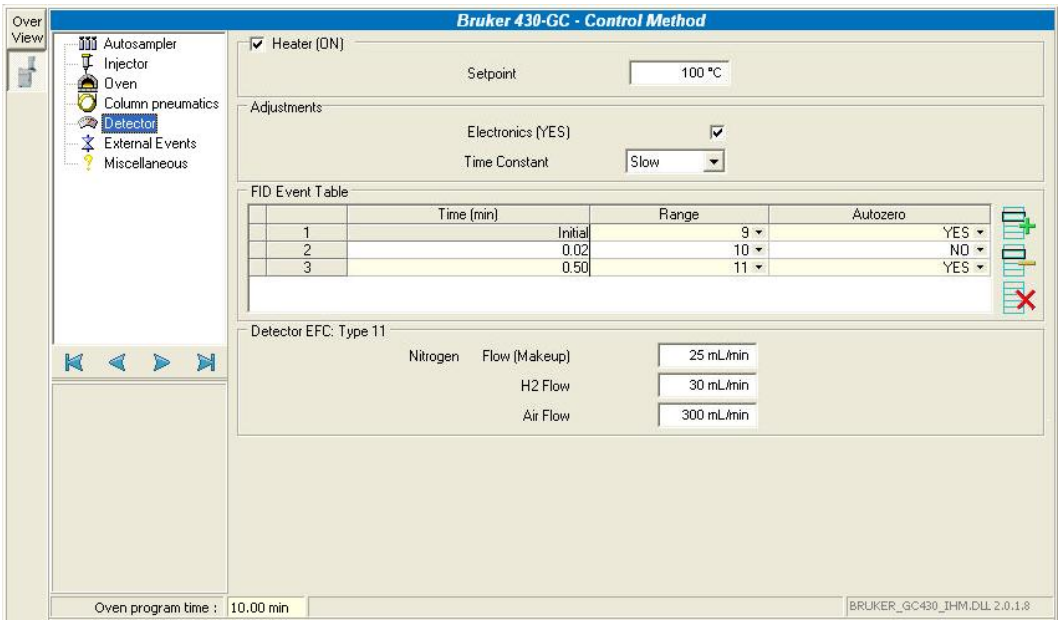
to delete a line in the table.

to clear the entire table.

Detector Control

The Detector sub-section allows you to specify the operating temperatures, gas flow rates, and specific parameters for the FID (Flame Ionization Detector) detector or the TCD (Thermal Conductivity Detector) detector.

FID Detector



Check or uncheck the Heater option to turn the detector oven ON or OFF and enter the detector oven temperature in the Setpoint field (50 to 450 °C).

Adjustments Parameter Group

Check or uncheck the Electronics option to indicate whether the installed FID will be used or not. Select the required Time Constant from the list (Fast or Slow).

FID Event Table Parameter Group

Use the spreadsheet to change detector settings during the analysis.

The first row of the spreadsheet contains the Initial Range and Autozero for the FID detector. When the autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The rest of the spreadsheet contains the time-programmed settings: the Range (9, 10, 11, or 12) and Autozero (Yes or No) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min)

Use the following buttons to edit the FID event table:

to add a line to the table.

to delete a line in the table.

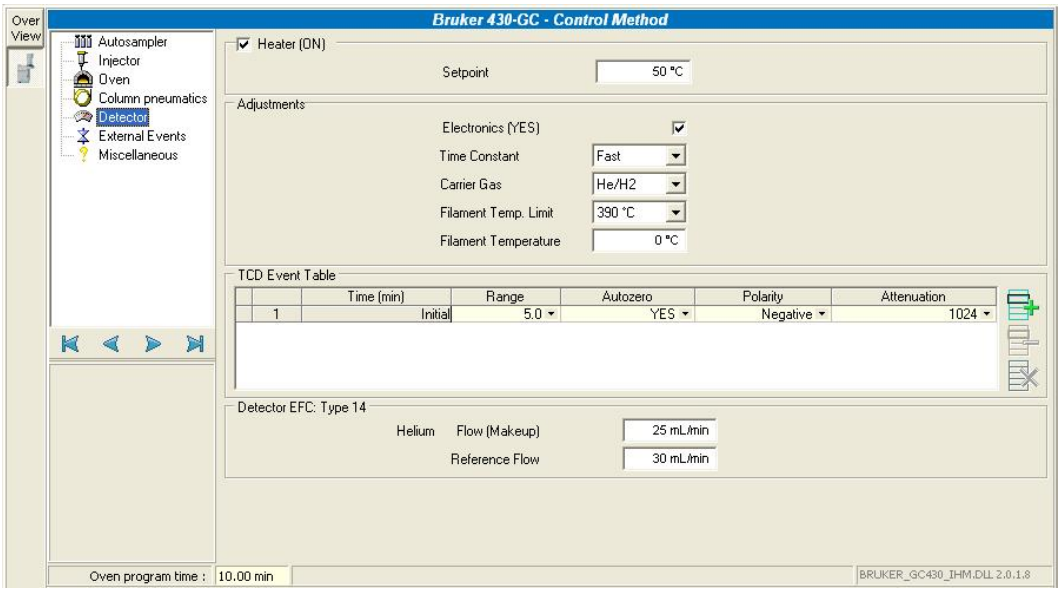
to clear the entire table.

Detector EFC Parameter Group

The Type 11 EFC section allows you to define the desired gas flow rates (Helium Flow (Makeup), H2 Flow and Air Flow fields, 0 to 50 mL/min for the makeup and hydrogen flows, and 0 to 500 mL/min for the air flow).

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For FID detectors, the EFC Type 11 is required.

TCD Detector



Check or uncheck the Heater option to turn the detector oven ON or OFF and enter the detector oven temperature in the Setpoint field (50 to 450 °C).

Adjustments Parameter Group

Check or uncheck the Electronics option to indicate whether the installed TCD will be used or not. Select the required Time Constant from the list (Slow or Fast).

Choose the Carrier Gas: if you are using helium or hydrogen as carrier gas, select the He/H2 setting. For all other carrier gases, select the N2/Ar setting.

Specify the Filament Temperature in the corresponding field (0°C to the maximum filament temperature) and select the Filament Temperature Limit from the list: to protect the filament, always operate the detector with the 390 °C limit selected unless you require the maximum dynamic range available to the TCD. With the limit set to 390 °C, the peak sample filament temperature is limited to approximately 450 °C. The temperature limit is approximately 550 °C at the 490 °C setting. The 450 °C limit protects filaments from oxidation when exposed to air over an extended period of time. However, at the 550 °C temperature limit the filament can degrade after only a few minutes.

TCD Event Table Parameter Group

Use the spreadsheet to change detector settings during the analysis.

The first row of the spreadsheet contains the Initial Range, Autozero and Polarity for the TCD detector. When the autozero is set to yes, it means the detector autozero is on continuous before the run starts. The polarity is used to reverse the peaks that appear in the negative direction (for example, if you inject a standard or sample into the reference side of the TCD).

The rest of the spreadsheet contains the time-programmed settings: the Range (0.05, 0.5 or 5.0), Autozero (Yes or No) and Polarity (Positive or Negative) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min).

NOTE: If you are also collecting the detector analog signal (via an analog output connected to a MIB-interface for example), you can define the required Initial Attenuation and change it during the analysis.

Use the following buttons to edit the TCD event table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

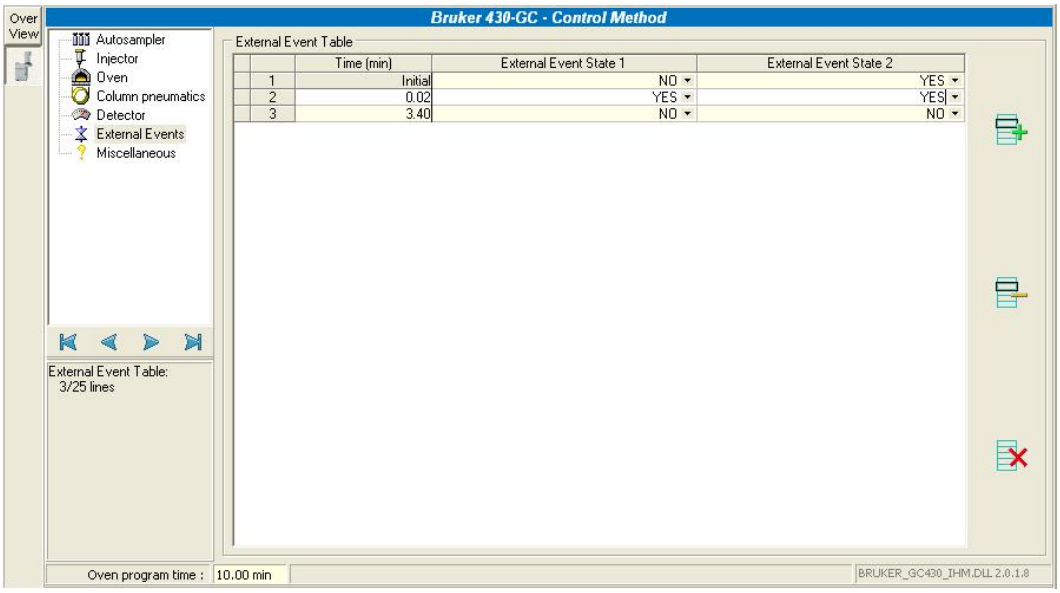
Detector EFC Parameter Group

If the detector Electronic Flow Control module is installed, the Type 14 EFC section will appear and allows you to define the desired gas flow rates (Makeup Flow and Reference Flow fields, 0 to 50 mL/min).

NOTE: The Electronic Flow Control modules (EFC) are detector-specific. For TCD detectors, The EFC Type 14 is required.

External Events Control

The 430 GC can have up to two external events:



External Event Table Parameter Group

Use the spreadsheet to time program the external events. The first row of the spreadsheet contains the initial external events position. The External Event State 1 and External Event State 2 columns allow you to turn the relay associated with each external event ON (Yes) or OFF (No). :

Use the following buttons to edit the External Events table

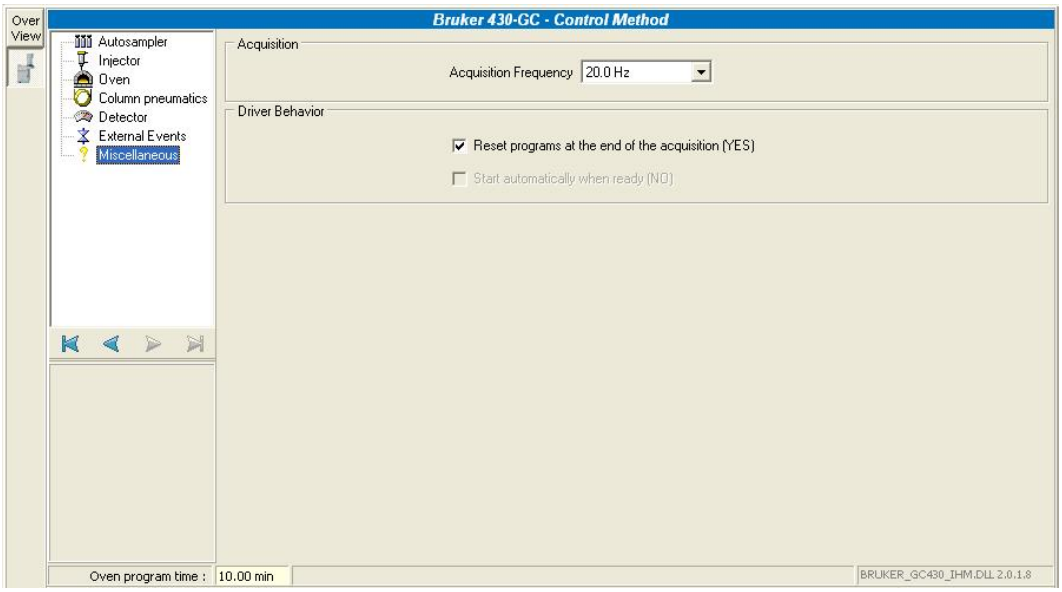
to add a line to the table.

to delete a line in the table.

to clear the entire table.

Miscellaneous Control

The Miscellaneous section contains parameters for data collection:



Acquisition Parameter

Enter the detector data rate in the Acquisition Frequency field. With decreased data rates, less disk space is required for storing the data. With increased rates, more data is collected, which may improve quantitation, particularly for narrow peaks.

Driver Behavior Parameter Group

Check or uncheck the Reset programs at the end of the acquisition to activate or deactivate this option. If it is checked and the acquisition is stopped from the acquisition window, the temperature programs will be reset before continuing with the next injection (if a sequence is running).

Check Start automatically when ready to start the GC without injecting. It could be useful in case of sampling valve use.

Starting and Viewing an Acquisition

Quick Start and Sequence

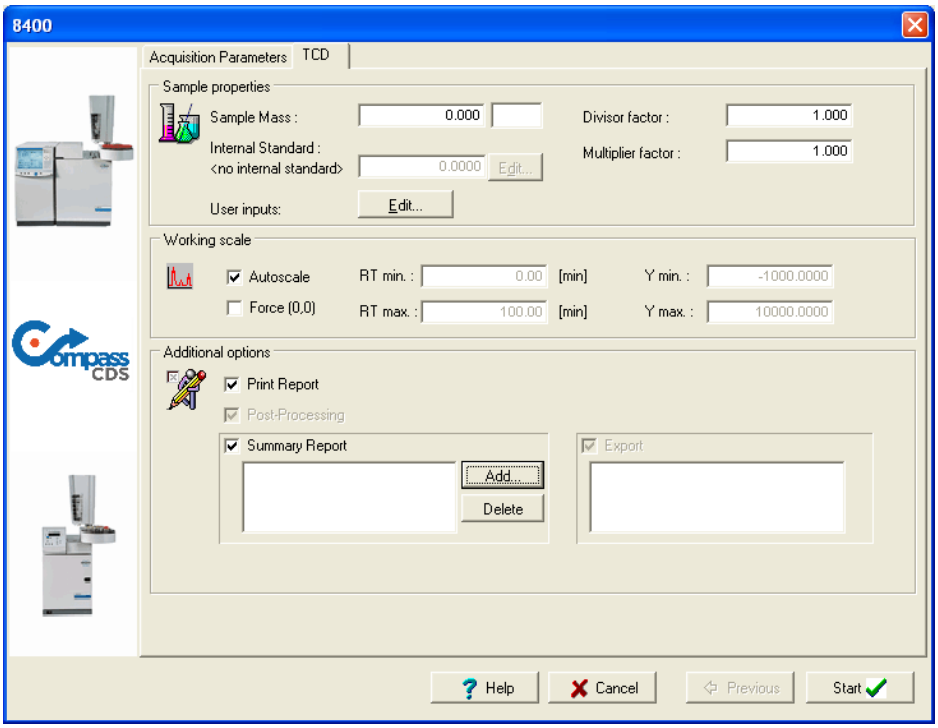
Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

Quick Start (Single Acquisition)

1. Press the button.

   In the Quick Start window, select the system, the method, and optionally the project if connected in "All project" mode.

2. Press the OK button. The following screen is displayed:



   In the Acquisition parameters tab, required fields like the Run Name, the Run ID and the Acquisition Run length must be filled before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by CompassCDS, the Injection Volume, the Vial position and the Rack number (if required) must be entered.

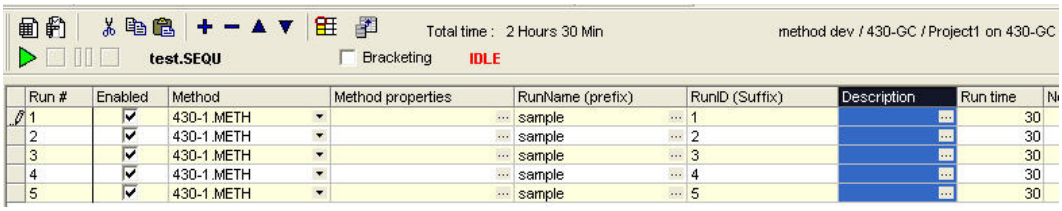
   Other parameters associated with each acquisition channel can be entered in the Channel X tab.

3. Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples) and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time
1	☑	430-1.METH		sample	1		30
2	☑	430-1.METH		sample	2		30
3	☑	430-1.METH		sample	3		30
4	☑	430-1.METH		sample	4		30
5	☑	430-1.METH		sample	5		30

The Method Name, the Run Name, the Run ID and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

To view a running acquisition, click on the Systems tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed. If Dual View is selected then the acquisition will be observed while the sequence is running.

Status of the 430 GC

Click on the button corresponding to the 430 GC driver and the 430 GC status screen will appear. It contains eight sub-sections: Autosampler, Injector, Oven, Column, Detector, External Events, Miscellaneous, and Overview. Click on the required sub-section to display the corresponding parameters that will be used during the chromatographic run.

A toolbar allows you to easily scroll through the status windows:

to select the first status window.

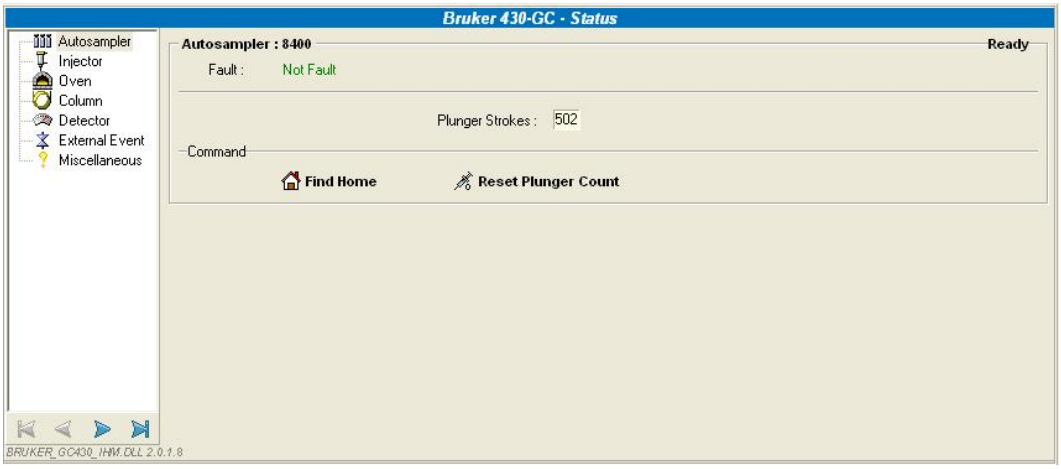
to move back to the previous status window.

to move forward to the next status window.

to select the final status window.

Autosampler Window

This section is only shown when 430 GCs have either an 8400 Autosampler or an 8410 AutoInjector connected to them.



The autosampler status screen indicates the autosampler state (Ready, Homing, Sampling or Running).

Fault or No Fault: displays if a fault in the autosampler component has occurred. In this case, a new button appears:

. Click on it to clear the fault.

Plunger Strokes: displays the number of times that the syringe plunger has been moved up and down. This can be used to help monitor syringe wear and plan for syringe replacements.

Click on the

button to reset the number of plunger strokes.

Click on the

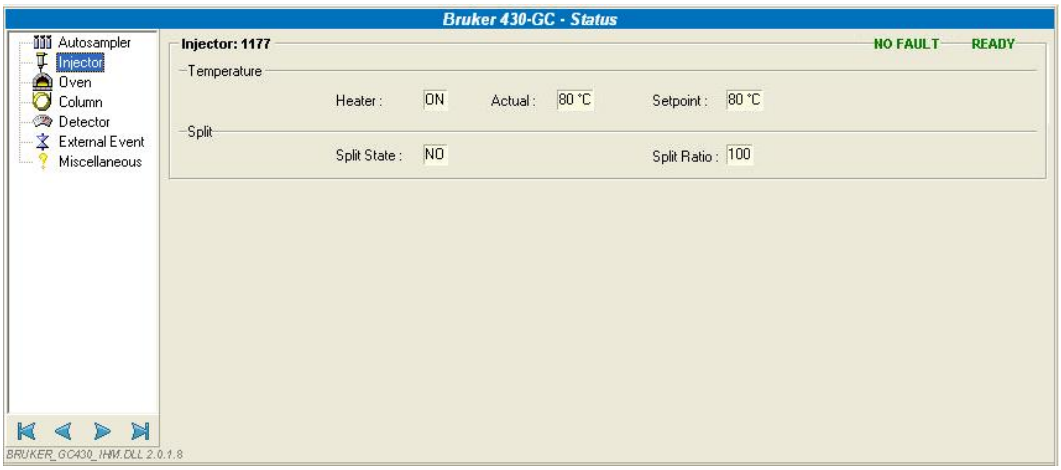
button to reinitialize the autosampler.

If an 8410 Autosampler is connected, the button

becomes available. Click on it to detect the tray orientation (1 to 10, 11 to 16, or 17 to 21).

Injector Window

1177 Injector



The following status parameters are available:

Ready, Not Ready or OFF: the injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”. The injector oven is OFF when the heater is OFF

Fault or No Fault: displays if a fault in the injector component has occurred.

Heater: displays if the injector oven component is turned OFF or ON at the 430 GC.

Actual: displays the actual temperature of the injector oven at the 430 GC.

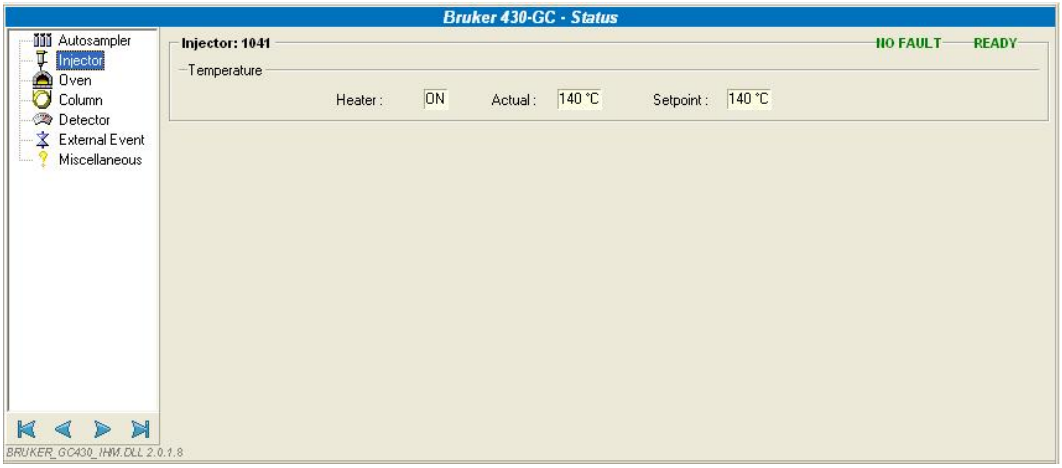
Setpoint: displays the injector oven programmed temperature setting in the active method. The 1177 injector is an isothermal injector.

Split State: displays the current split state of the 1177 injector method.

Split Ratio: displays the current split ratio of the 1177 injector method.

The split ratio is defined as the (Column Flow + Split Flow) / the Column Flow.

1041 Injector



The following status parameters are available:

Ready, Not Ready or OFF: the injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”. The injector oven is OFF when the heater is OFF

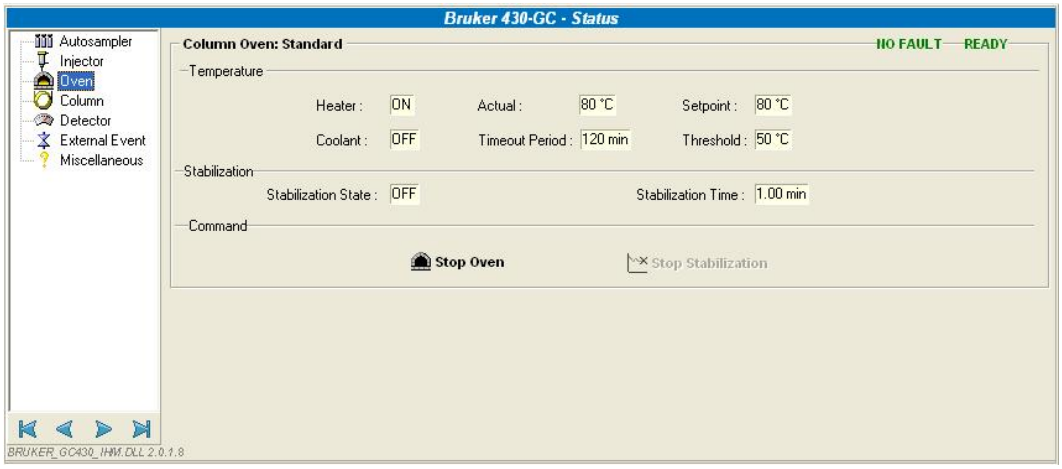
Fault or No Fault: displays if a fault in the injector component has occurred.

Heater: displays if the injector oven component is turned OFF or ON at the 430 GC.

Actual: displays the actual temperature of the injector oven at the 430 GC.

Setpoint: displays the injector oven programmed temperature setting in the active method.

Column Oven Window



The status display includes the following parameters:

Ready, Not Ready or OFF: the column oven is Ready if the setpoints have been achieved and stabilized. The column oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance. The column oven is OFF when the Heater is turned OFF.

NOTE: Some reasons the GC may display Not Ready during a run are: the temperature program is too aggressive, the oven door is opened, the coolant runs out, or the power line voltage drops.

Fault or Not Faulted: displays if a fault in the column oven component has occurred.

Heater: displays if the column oven component is turned OFF or ON at the 430 GC.

Actual: displays the actual temperature of the column oven at the 430 GC.

Setpoint: displays the column oven programmed temperature setting in the active method.

Coolant: displays if the column oven coolant is enabled in the active method.

Timeout Period: displays the programmed coolant time-out value in the active method for the column oven.

Threshold: displays the programmed column oven temperature at which the column oven coolant is enabled.

Stabilization State: displays the current stabilization state of the oven. When the state is ON, the button

becomes active. Click on it to bypass the stabilization time.

Stabilization Time: shows the 430 GC column oven stabilization time in minutes. The stabilization time counts down from the programmed method value and then displays 0.00 minutes when the stabilization period is over.

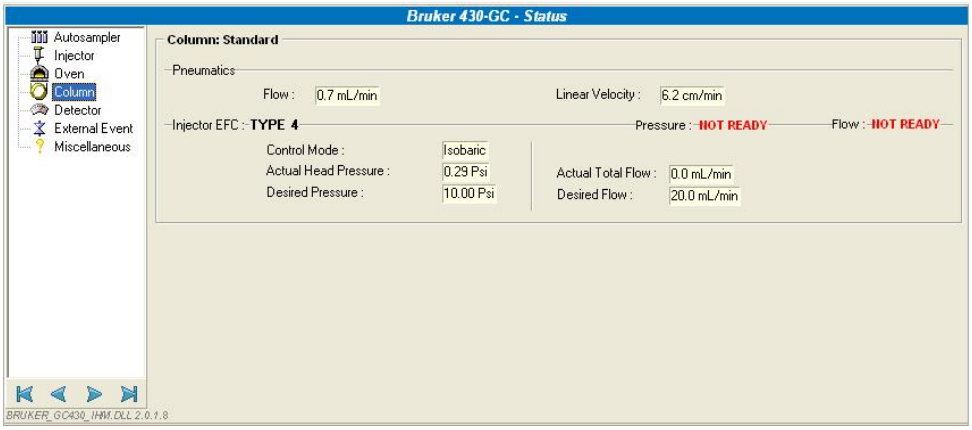
Click on

to turn off the oven when the oven is on.

Click on

to turn on the oven when the oven is off.

Column Window



The status display includes the following parameters:

Flow: displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Linear Velocity: displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

The injector EFC type is mentioned (Type 1 for 1177 injector, Type 4 for 1041 injector)

Pressure: Ready or Not ready. The Injector EFC pressure is Ready if the setpoint has been achieved and stabilized.

Flow: Ready or Not ready. The Injector EFC flow is Ready if the setpoint has been achieved and stabilized.

Control Mode: displays the control mode of the EFC (isobaric, constant flow).

Actual Head Pressure: displays the actual column head pressure at the 430 GC.

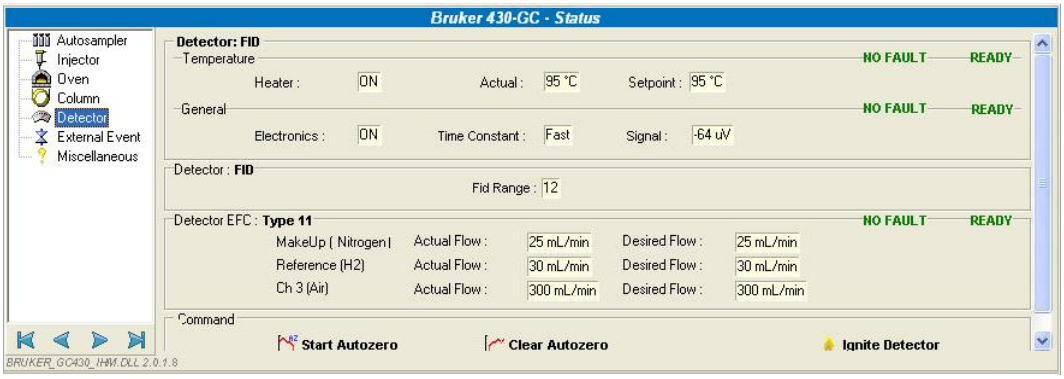
Desired Pressure: displays the programmed column head pressure setting in the active method.

Actual Total Flow: displays, in mL/min, the total flow rate through the system.

Desired Flow: displays the programmed column flow setting in the active method.

Detector Window

FID Detector



The status display includes the following parameters:

Temperature

Ready or Not Ready. The temperature of the FID detector is Ready if the setpoints have been achieved and stabilized.

Fault or No Fault. Displays if a fault in the FID detector component has occurred.

Heater: displays if the detector oven component is turned OFF or ON at the 430 GC.

Actual: displays the actual temperature of the detector oven at the 430 GC.

Setpoint: displays the detector oven programmed temperature setting in the active method.

General

Ready, Not Ready or OFF. The ready state is displayed if the setpoints for FID temperature and electronics have been achieved and stabilized. The Not ready state is displayed if temperature and electronics setpoint are not reached. The OFF state is displayed if the FID electronics are turned off.

Fault or No Fault. Displays if a fault in the FID detector component has occurred.

Electronics: displays the FID Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: displays, in mV, the actual FID detector signal at the 430 GC.

Detector

FID Range: 9, 10, 11, or 12. Displays the FID Range initial condition setting or the time-programmed setting in the active method.

If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and displays the following parameters:

Detector EFC

Ready or Not Ready. The Detector EFC is Ready if the setpoints have been achieved and stabilized.

Fault or No Fault: displays if a fault in the Detector EFC component has occurred.

Make Up: displays, in mL/min, the setpoint and actual channel 1 flow rate (Make up).

Reference: displays, in mL/min, the setpoint and actual channel 2 flow rate (Hydrogen).

Ch 3: displays, in mL/min, the setpoint and actual channel 3 flow rate (Air).

Command

Click on the

button to ignite the detector flame.

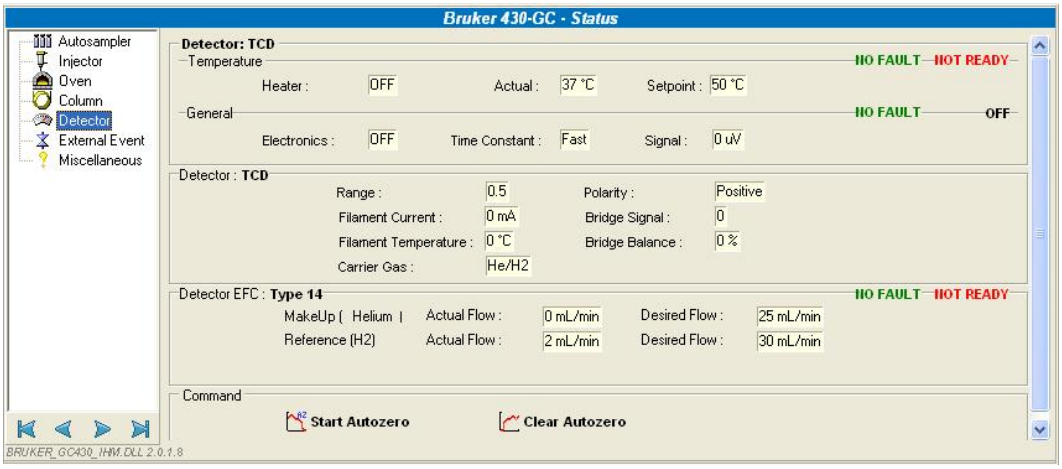
Click on the

button to launch the autozero of the detector.

Click on the

button to clear the autozero of the detector and get the raw signal from the detector (useful in case of diagnosis situation).

TCD Detector



Temperature

Ready or not ready: the TCD detector is Ready if the setpoints have been achieved and stabilized. The TCD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the TCD detector becomes not ready or goes “out of tolerance”.

Fault or No Fault: displays if a fault in the TCD detector component has occurred.

Heater: displays if the detector oven component is turned OFF or ON at the 430 GC.

Actual: displays the actual temperature of the detector oven at the 430 GC.

Setpoint: displays the detector oven programmed temperature setting in the active method.

General

Ready, Not Ready or OFF. The ready state is displayed if the setpoint for TCD temperature and electronics have been achieved and stabilized. The Not ready state is displayed if temperature and electronics setpoints have not been reached. The OFF state is displayed if the TCD electronics are turned off.

Fault or No Fault. Displays if a fault in the TCD detector component has occurred.

Electronics: displays the TCD Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: displays, in µV, the actual TCD detector signal at the 430 GC.

Detector

Range: 0.05, 0.5, or 5.0. Displays the TCD Range initial condition setting or the time-programmed setting in the active method.

Filament Current: displays, in mA, the actual TCD current.

Filament Temperature: displays the TCD Filament Temperature setting in the active method.

Carrier Gas: displays the carrier gas setting in the active method.

Polarity: displays the TCD polarity initial condition setting or time-programmed setting in the active method.

Bridge Signal: displays the actual TCD bridge signal.

Bridge Balance: displays the TCD bridge balance (%).

The Type 14 EFC section will display the following parameters:

Detector EFC

Ready or Not Ready. the detector EFC is Ready if the setpoints have been achieved and stabilized.

Fault or No Fault: displays if a fault in the detector EFC component has occurred.

Make Up: displays, in mL/min, the setpoint and actual channel 1 flow rate.

Reference: displays, in mL/min, the setpoint and actual channel 2 flow rate.

Command:

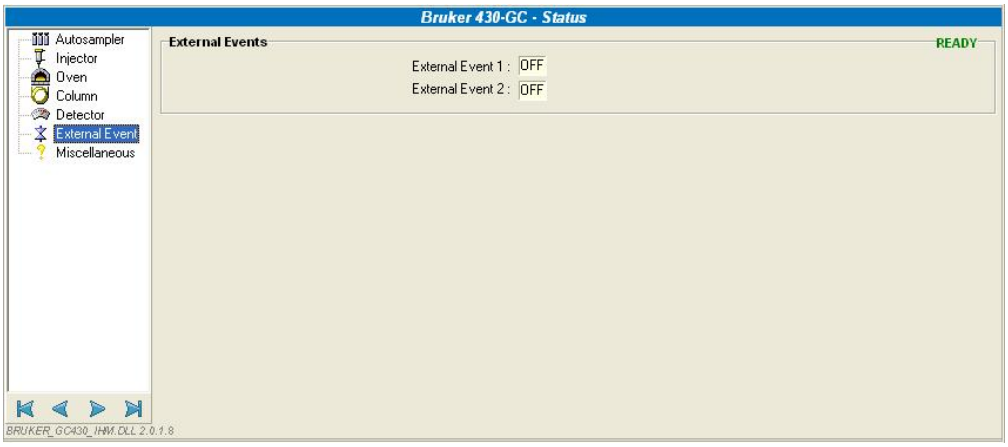
Click on the

button to launch the autozero of the detector.

Click on the

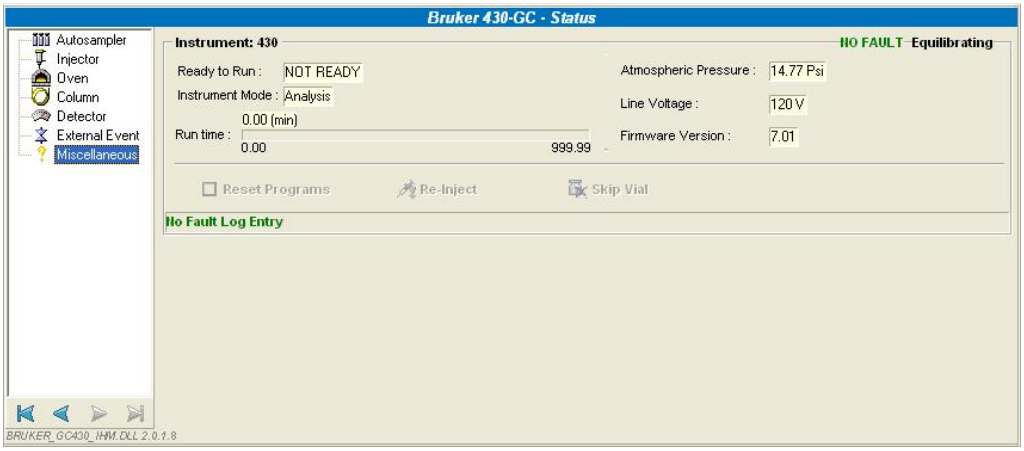
button to clear the autozero of the detector and get the raw signal from the detector (useful in case of diagnosis situation).

External Events Window



The status screen displays the current state of each external event.

Miscellaneous Window:



The miscellaneous screen contains general information about the current run, the overall state of the instrument and the GC Firmware Version.

The state of the instrument (Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready) is displayed.

A Fault / No Fault indicator is also shown. When a hazardous or disabling fault occurs, any run in progress will halt and the affected component will shut down. If the fault is recoverable, then the run is not terminated.

The run time bar displays the elapsed time in minutes since the beginning of the run and the end time.

Atmospheric Pressure: displays the current value of the atmospheric pressure calculated by the GC.

Press the

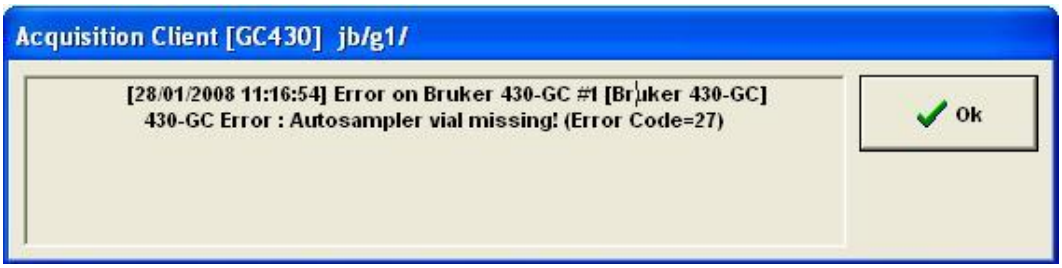
button, to reset the GC. If it is RUNNING, the GC aborts the current run, goes to the READY state and continues with the next injection in the sequence. This button is equivalent to pressing the Stop on the front panel of the GC.

When a vial is missing during a sequence, a warning message appears and you have 10 minutes to replace the sample in the correct position before the system skips the missing vial and passes to the next line of the sequence, or stops the run. When you have replaced the missing sample, you must press the

button to restart the run.

If you want to skip the missing vial and start the next run, you must press the

button.


Acquisition Client [GC430] jb/g1/
[28/01/2008 11:16:54] Error on Bruker 430-GC #1 [Bruker 430-GC]
430-GC Error : Autosampler vial missing! (Error Code=27)
Ok

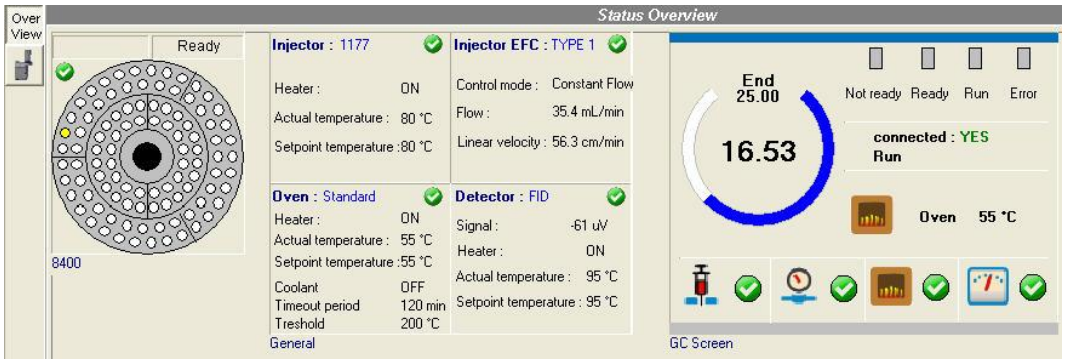
Warning message when a vial is missing.

Overview Window

Click on the Over View button: the Status Overview window is displayed and contains three tabs:

General

Displays the synopsis of the instrument, where some current values can be read (temperatures, pressures, and signal).



When the mouse points to a colored vial (yellow for current vial, green for already used vial and red for missing vial), the current vial number and the number of injections are displayed.

The flow and temperature (current and setpoint) for each module and the signal values are displayed. You can choose to display the flow, the pressure or the velocity of the gas in the column by clicking on the button.

Not Ready

Contains the not ready information sent by the instrument.

Events

Contains the events that have occurred on the instrument, listed below:

430 GC Faults

-5V / +5V out of range	The –5V / +5V power lines are outside of their allowed tolerance for correct GC operation.
ADC Calibration failure	Activate a method to clear this fault. If the fault recurs, turn the GC off and then on.
Board Failure	The 430 GC just detected that the specified detector has a failed electronics board.
DAC Calibration failure	The DAC (Digital to Analog Converter) that supplies the analog output signal failed to calibrate within its set tolerance. Turn off the power and then turn it back on.
DIAG Temp. out of range	The actual temperature of a temperature controlled resistor block used for automatic instrument calibration has exceeded its allowed temperature set point. Turn the power to the GC off and then on again.
Fan unplugged during run	Turn off instrument and turn it back on.
FID Flame out	The FID flame has been quenched. The flame detection is based on a background signal intensity of approximately 330 microvolts. It is possible for very clean GC systems to have baselines less than 330 microvolts causing spurious flameout messages. If you suspect that the flameout message is spurious, use a shiny, cool metal object (such as a box end wrench) and hold it just above the FID tower being careful not to get too close to the hot surfaces. If you observe condensation then the flame is still lit; you may wish to change your fuel gas mixture or some other operating characteristic that would allow a slightly higher background signal. Once a flame out is detected, the system will attempt to ignite the flame 3 times before reporting the flame out condition. The fault is cleared by either igniting the flame using the Ignite FID Flame! Command or by turning the Detector electronics off and then on again.
Gas saver timeout expired	The GC has been idle for a period of time equal to or greater than the set Gas Saver timeout period. Activate a method to clear the fault.
Internal Temp. limit exceed	Turn off instrument and turn it back on.
IOP Communication failure	Turn on the instrument off then on again.
Lower than minimum temp	The 430 GC just detected that the specified component temperature zone has gone below its minimum temp.
Max setup temperature limit exceeded	The 430 GC just detected that the specified limit exceeded component temperature zone has exceeded its maximum setup temperature limit.
Maximum temp has been exceeded	The 430 GC just detected that the specified component temperature zone has exceeded its maximum temperature.
Step motor moving	The column oven vent stepper motor has failed to reach its internally set position within the step tolerance. Turn the power off and then on again
Temp probe is open	The 430 GC just detected that the specified component temperature zone probe has an open circuit.
Temp probe is shorted	The 430 GC just detected that the specified component temperature zone probe has a short circuit.
Temp probe response is too fast	The 430 GC just detected that the specified component temperature zone probe is responding too fast.
Temp probe response is too slow	The 430 GC just detected that the specified component temperature zone probe is responding too slowly.
Thermal runaway	The 430 GC just detected that the specified component temperature zone has begun thermal runaway.

Autosampler Faults

84x0 communication	The AutoSampler/AutoInjector has experienced an error during communications that was unrecoverable. Power off both the GC and the autosampler. Turn on power to the GC followed by turning on the power to the autosampler.
84x0 faulted	The rautosampler has failed to properly initialize. Turn off the power and then turn it back on
84x0 carousel error	The autosampler carousel base has encountered one or more internal faults and has failed to properly come up. Turn off the power and then turn it back on.
84x0 carousel sensor not found	The autosampler carousel sensor has failed to conform to its expected operation. Turn off the GC and then on again.
84x0 maximum plunger speed exceeded	This message is displayed if you have built a method with one syringe that supports a fast injection speed and have subsequently changed and configured a different syringe. Correct the syringe speed in your method for the new syringe
84x0 plunger error	The syringe plunger has either jammed or become inoperable. Check that the syringe is properly mounted and that you have free movement of the plunger. Replace the syringe if required.
84x0 plunger strokes exceeded limit	This is an advisory message that the plunger limit stroke count has exceeded the limit that was set for it. You should change the syringe and zero the plunger stroke counter soon after you observe this message.
84x0 plunger sensor not found	The autosampler plunger sensor has failed to conform to its expected operation. Turn off the GC and then on again.
84x0 run not started after injection	Restart Automation to clear this fault. If it recurs, check that the inject switch installed on the injector nut is functioning properly.
Run ended before injection	The autosampler failed to complete the injection sequence. Restart a run to clear the fault
84x0 syringe sled sensor not found	The syringe sled is either jammed or miscalibrated. Recalibrate your vial and injector positions making sure that the syringe sled has a small clearance (consult your manual) above vials and does not compress the injector switch on the injector.
84x0 syringe volume exceeded	The total volume of the sample, air gaps (if any), solvent plugs (if any), and internal standards (if any) exceeds the capacity of the configured syringe. Note that this error is only sensed at the time of injection. Check your method and correct any volumes that are excessive.
84x0 syringe missing	The autosampler has sensed that the syringe is not installed. Check that you have a syringe installed.
84x0 tower error	The autosampler tower has one or more internal faults and has failed to properly come up. Turn off the power and then turn it back on.
84x0 tower sensor not found	The tower sensor does not conform to its expected operation. Turn the GC off and then on again.
84x0 tray is missing	The 8410 sample tray has been removed from the base. Replace the tray; the 8410 should automatically sense that the tray has been replaced.
84x0 vial missing	The autosampler has failed to detect a vial within an expected range of vials. This message is an advisory message. If you have a vial in the position and it has been missed, check that a septum is installed. Lack of a septum and dark colors may cause the tower sensor to fail to identify the vial.
84x0 vial sensor bad	The autosampler vial sensor has failed to conform to its expected operation. Turn the GC off then on again..
8410 Vial is unreachable	This message informs you that the 8410 tray is oriented such that the requested sample vial does not fall under the arc of the tower. Re-orient the tray or change the requested vial from which you intend to inject to correct this.

Varian 3800 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501492
Revision D

Contents

Introduction 3
General 3
Installation and Configuration 3
Installing the Driver Software 3
Configuring the GC Communications 3
Ethernet Communications 3
Configuring the Driver 4
Configuring the 3800 GC 4
Configuring the Synopsis 6
Building a Method 8
Creating a New Method 8
3800 GC Control Method Section 10
Autosampler Control 11
Injectors Control 23
Column Oven Control 29
Column Pneumatics Control 30
Detectors Control 35
Output Ports Control 45
Valves Control 46
Miscellaneous 49
Starting and Viewing an Acquisition 51
Quick Start and Sequence 51
Quick Start (Single Acquisition) 51
Sequence 52
Running Acquisition Status 52
Viewing a Running Acquisition 52
Status of the 3800 GC 52

Introduction

General

This document describes the configuration of the Varian 3800 GC driver. It also explains how to build a control method for this driver, how to start and view a running acquisition, and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

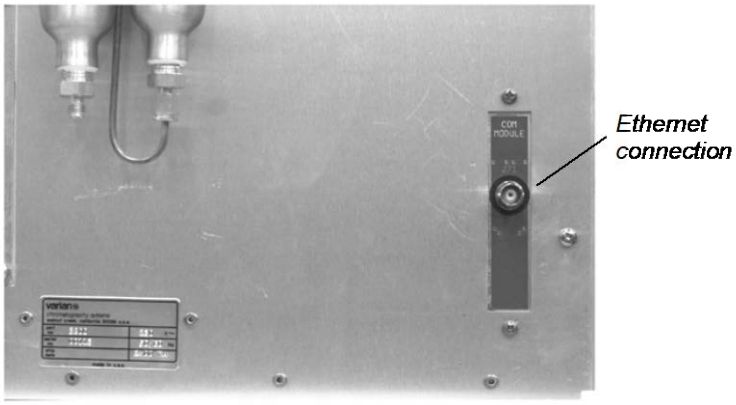
To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

Configuring the GC Communications

Ethernet Communications

The 3800 GC Gas Chromatograph uses Ethernet® as the method of communications for instrument control.

The optional 3800 GC Communications Board has a 10Base2 Ethernet connector located on the rear of the GC. This BNC style connector accepts RG58C/U cable connections. The standard 3800 Communications kit contains a six foot cable and a BNC Tee. The BNC Tee is connected to the GC BNC connector. The Ethernet cable connects the BNC Tee on the 3800 GC to the CompassCDS Workstation Ethernet board or to a cable or switch on a company network.



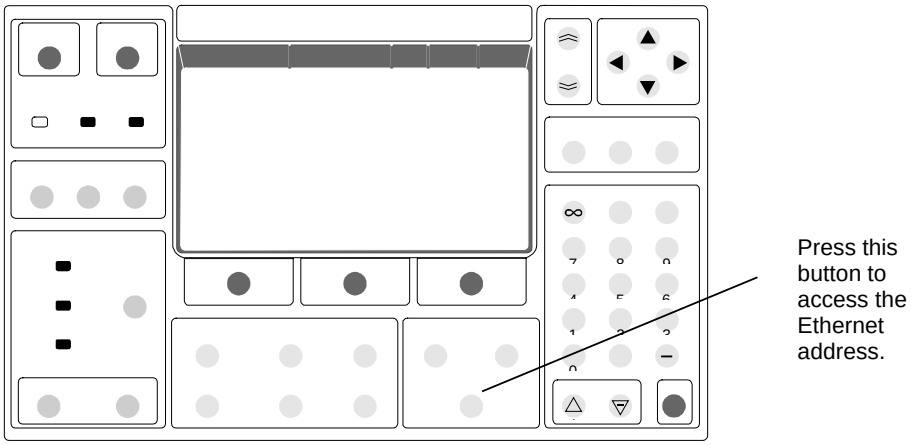
The 3800 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server is used to send IP addresses to TCP/IP devices. A static IP address can be configured in the GC but only if the instrument has firmware 3.3.5 or greater.

The BOOTP Server lists Ethernet addresses along with the IP addresses that are to be assigned to the corresponding devices.

To know how to configure the BOOTP server, refer to the CompassCDS Installation Guide.

NOTE: To find the Ethernet address of the 3800 GC, turn on the GC and, when prompted, press any key to allow it to start in local mode. When the GC has completed its initialization process, press the Menu button and press 1 to select the Remote /Local Control screen. The Ethernet address is displayed. This procedure prevents communication between the GC and the BOOTP server, so no IP address or Host name will be assigned to the GC until it is rebooted and allowed to contact the BOOTP server.



NOTE: The BOOTP server provided by the CompassCDS Chromatography Data System is installed during the installation of the CompassCDS software.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the 3800 GC

Click on the button corresponding to the 3800 GC driver and the GC configuration screen appears.

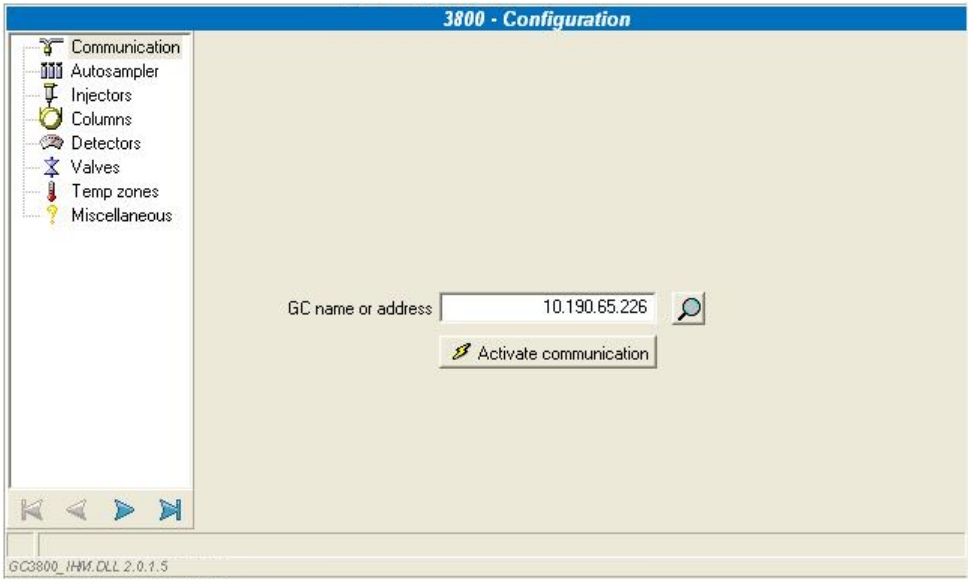
The toolbar allows you to easily scroll through the configuration windows:

To select the first configuration window.

To select the previous configuration window.

To select the next configuration window.

To select the final configuration window.



Select the ‘Communication’ sub-section and enter the IP address of the 3800 GC (configured in the BOOTP server) or click on the button to find the instrument previously configured with the BOOTP server program and select it.

Press the

button to automatically get the configuration from the instrument.

Select the following sub-sections to see the corresponding module configurations (the screens displayed are read-only screens):

Autosampler: Displays the autosampler type if installed, the autosampler position, the number of injection ports, the syringe volume or type.

Injectors: Displays, for each injector identified by its location (Front, Middle, Rear), the injector type, the installed temperature zone, the associated injector EFC type if installed, the outlet pressure, the pressure display units, the splitless vent flow, the gas saver flow, the gas saver timeout, the column septum purge head pressure and the septum purge flow rate.

Columns: Displays whether the column is installed or not (the location -Front, Middle, or Rear- refers to the sample introduction device to which the column is connected), the corresponding temperature zone and the column parameters, which include the carrier gas, the capillary column length and ID (Inside Diameter). If a packed column is used, then 0 is set for length and ID. The carrier gas and column dimension information is used for EFC calculations.

Detectors: Displays the detector type for each location (Front, Middle, Rear), the corresponding temperature zone, the corresponding EFC type if installed, and the channel 1, 2, 3 gas types according to the installed EFC. If an FID electrometer is installed, the *Check for FID flameout* parameter allows the GC to ignore flameout test results. This could be used if you have a very low background system, or when the FID electrometer is used to collect signal from another low-background detector, such as a PID. The *Micro-TCD resistance* (Ohm) field displays the filament resistance of the installed cell. The GC uses this value to calculate proper filament current.

Valves: Displays the name of the installed valves. Seven external events are available on the 3800 GC. When a name has been chosen in the instrument setup, this also defines the default states of the valve. These states will be visible when the valve is being programmed in the valve control section of the 3800 GC method.

Temp zones: Displays the six available heated zones on the 3800 GC and the column oven heated zone. All zones have temperature programming capability and three (Coolable zones 1 - 3) have cryogenic cooling capability. Typically, Coolable zones 1 - 3 are assigned to injectors and Heat-only zones 1 - 3 to detectors.

Miscellaneous: Displays the date format and language. The '*Is ready' in a closed contact* parameter displays what switch state corresponds to External Device Ready.

NOTE: If you want to modify the GC configuration, you need to use the Setup button directly on the instrument front panel. The 3800 GC is configured at the factory, and you need to enter Setup only when hardware is being installed such as a column or a field upgrade is done or an option is removed. Refer to the instrument manual for more details.

Configuring the Synopsis

In the *Overview* part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

1. To save the configuration of these devices, click on the *OK* button.

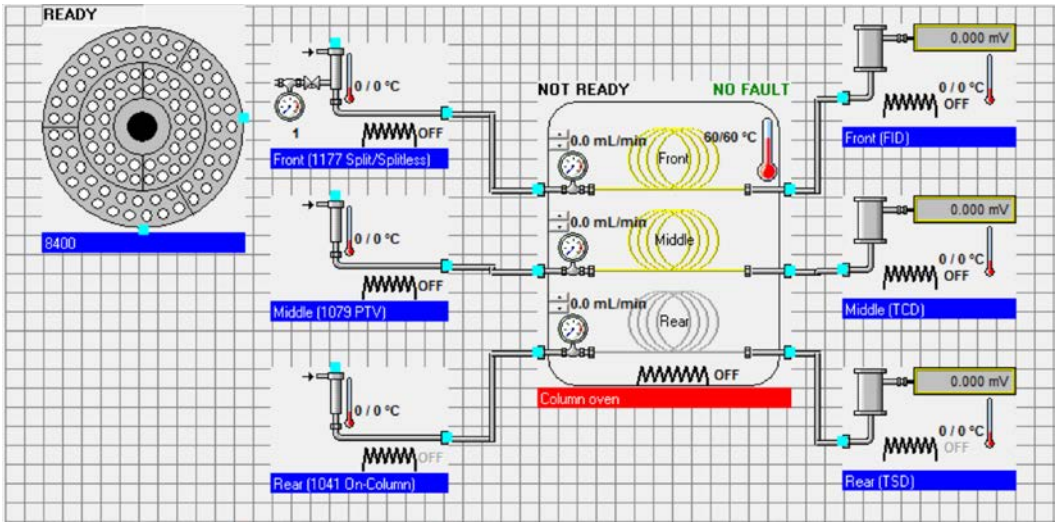
2. Right click on the system name in the bottom part of the *CompassCDS Configuration Manager* screen. A pop-up menu appears: click on *Stop.* Then right click on the system name again, and click on *Start*.

3. Go back to the System Configuration screen (Properties wizard). A graphic of the devices that comprise the system, is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, and connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

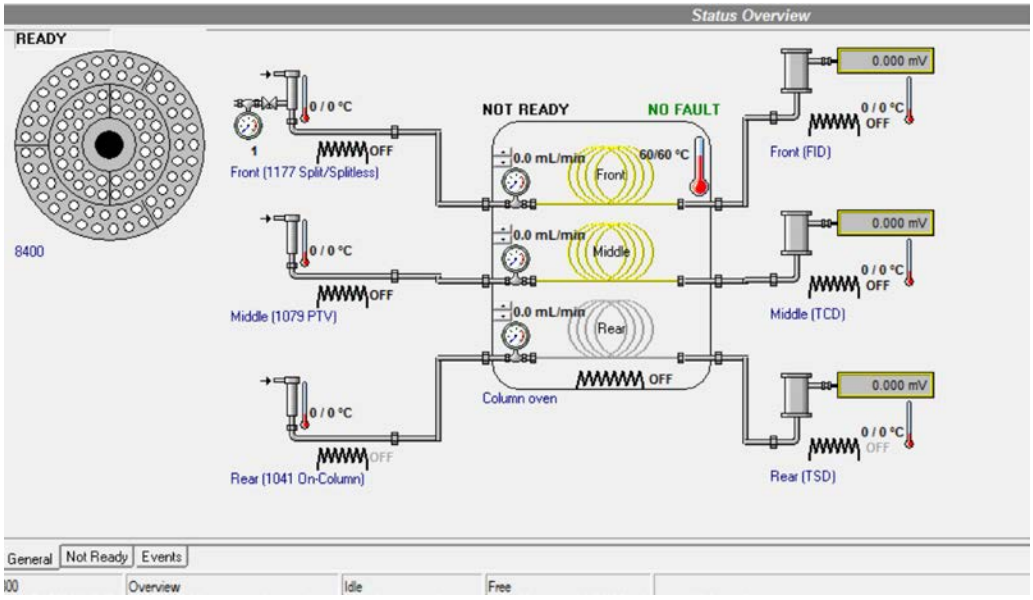
   Click on the to delete a selected tube; click on the button to delete all the tubes.
   Click on to define a background color, or on to make the background transparent.
   Click on the icon to change the grid color.

4. Once the synopsis configuration is complete, it will be displayed in CompassCDS, in the Systems tab. In this tab, the Overview part will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.) depending on the installed devices.

   For example, the following pictures represent the synopsis of the 3800 GC:



CompassCDS Configuration Manager Screen



CompassCDS screen

NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Click on the button to print the current configuration

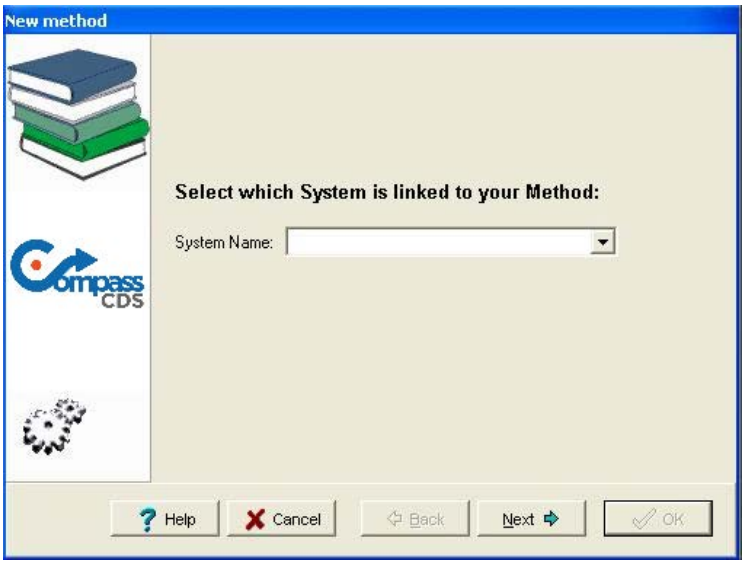
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument section prior to starting an acquisition.

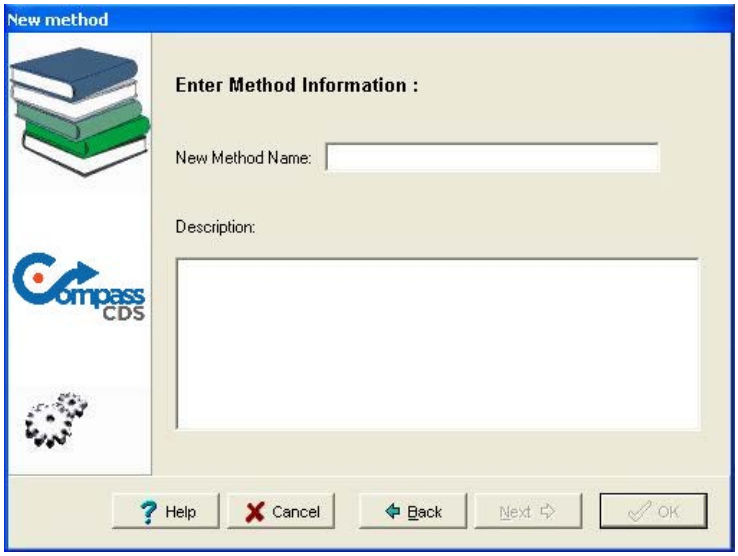
1. To create a new method, select the *FILE / NEW METHOD* option from CompassCDS main menu.

A wizard guide will appear and provide assistance during the first steps of method creation:



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

3. Once this field is completed, click on the Next button to move to the second step of the method creation:



4. Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

5. Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in CompassCDS. The next step is the definition of each of the method sections.

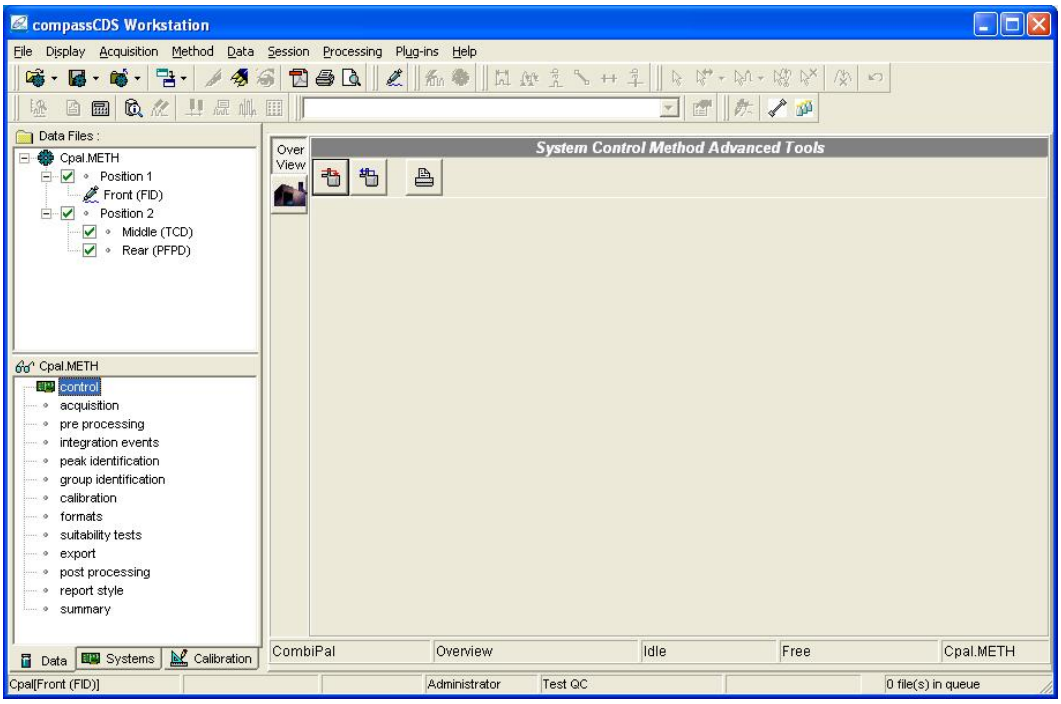
The instrument *control* section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the 3800 GC is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, refer to CompassCDS User Guide.

3800 GC Control Method Section

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



Press the Over View button to display the *System Control Method Advanced Tools* window:

To send the current method to the instrument.

To get the active method from the instrument.

To print the current method.

Click on the button to display the 3800 GC control method section. It contains eight sub-sections: *Autosampler*, *Injectors*, *Column oven*, *Column pneumatics*, *Detectors*, *Output ports*, *Valves*, and *Miscellaneous*. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

The toolbar allows you to easily scroll through the control method windows:

To select the first window of the control method.

To move back to the previous window of the control method.

To move forward to the next window of the control method.

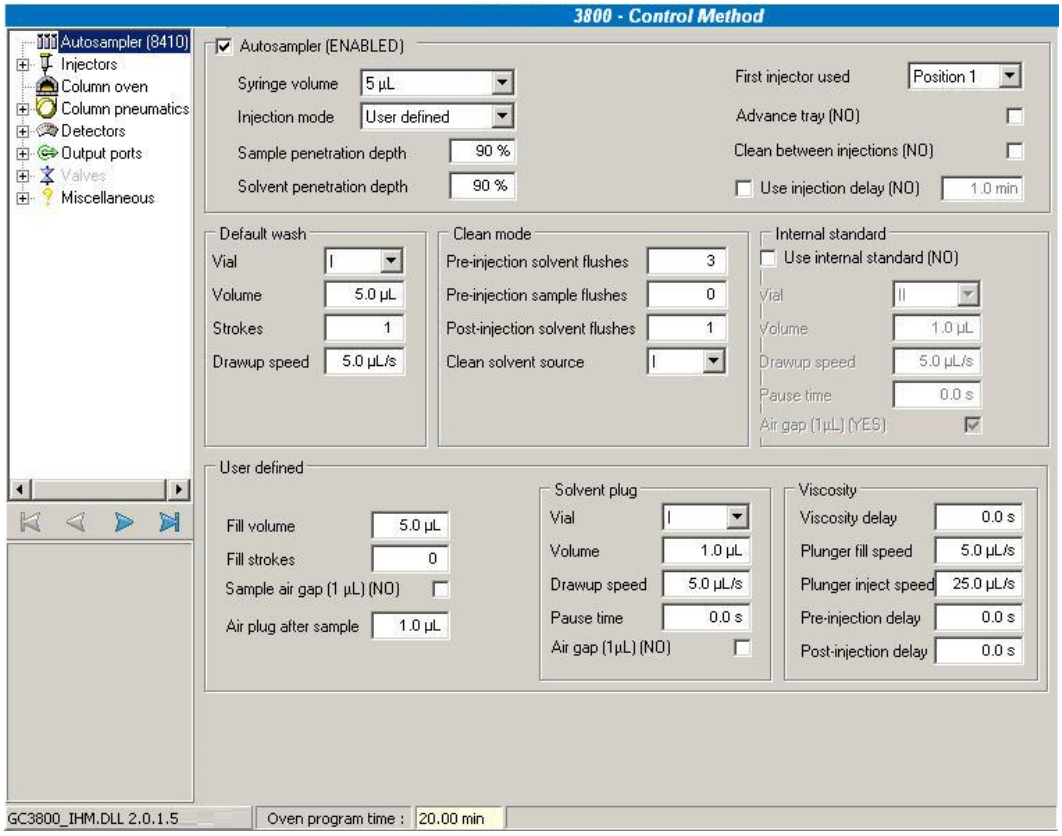
To select the final window of the control method.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Autosampler Control

The autosampler window contains sampling parameters for the 8400/8410 AutoSampler when attached to the 3800 GC:

Liquid Mode



Autosampler Parameter Group

In this parameter group, define the sampling syringe size, the penetration depth for sample and solvent wash vials, the injection mode, and injector position.

Dual and Duplicate injections using the 3800 GC with two injectors, the 8400/8410 AutoSampler and CompassCDS

The CompassCDS software will support the 8400 Dual and Duplicate modes of operation on the 3800 GC appropriately equipped with two injectors. Dual injection mode allows an operator to inject samples from two adjacent vials into both a front and back injector that lies on the arc of the

8400/8410 tower. Duplicate mode injections allow an operator to inject aliquots from the same vial into both injectors as described above. In order to use these features, you must perform certain steps for both the 3800/8400 setup and for CompassCDS.

Configuring the 3800/8400/8410

CompassCDS will read the configuration from the GC and will use it to configure itself to either use one injector only, or to allow dual and duplicate injections as well as single injections. To configure the 3800 for dual and duplicate injections:

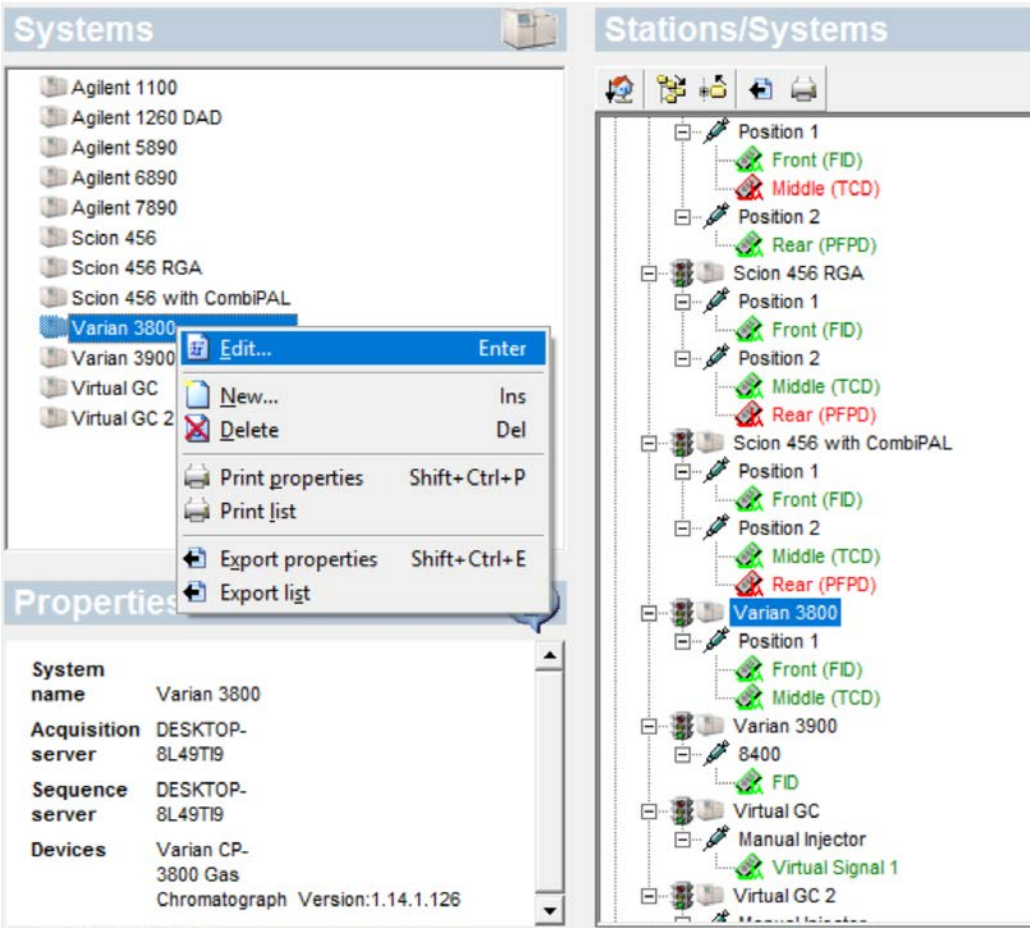
- Press the Setup key on the 3800 keyboard
- Select [2] Edit Instrument Setup
- Select [5] Edit Sample Delivery Parameters
- Select [1] Edit CP-8400/8410 Setup
- Set the Injector Ports to Use With 8400/8410 to Both
- Save and Exit Setup; the 3800 will reboot.

It is assumed that you have calibrated the CP-8400/8410 for both the front and back injector positions that you will be using. If you have not done this, you should make certain the calibration is done before you start using your system.

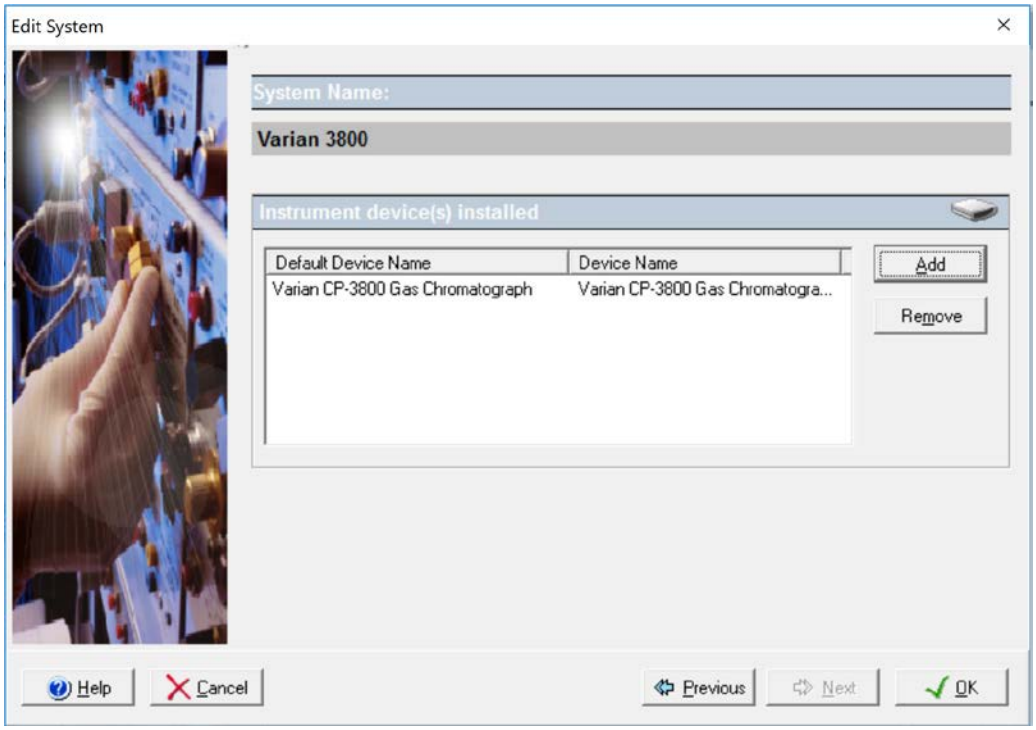
Configuring CompassCDS

In order to configure CompassCDS you will first have to add the instrument you are using if you have not already done so.

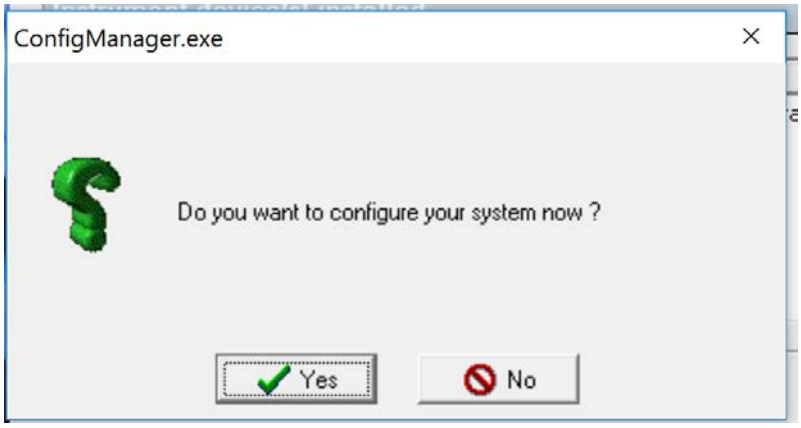
Follow the instructions in the CompassCDS Manuals for creating a new instrument. If you already have an instrument right-click on the instrument and choose edit….; follow the instructions below.



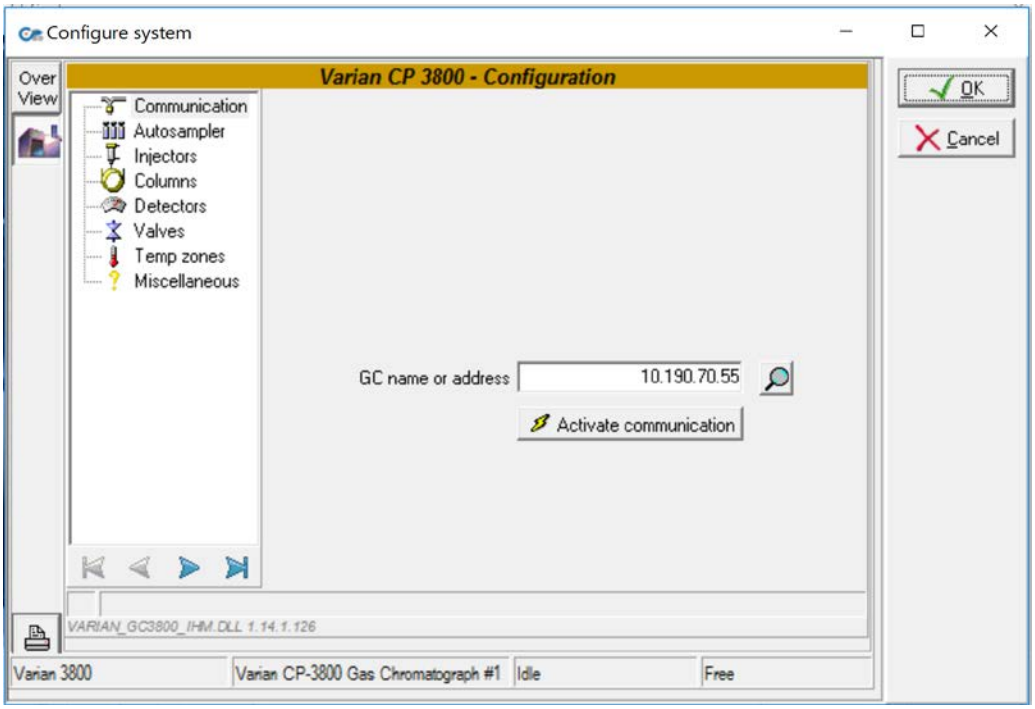
Click on the *Next* button at the bottom of the CompassCDS screens until you obtain the following screen. Click on the *OK* button to configure the system



The following screen is displayed after you click on *OK*. Click on the *Yes* button.



Click on the 3800 GC Configuration icon and check to make sure that the configuration has been received from the instrument.

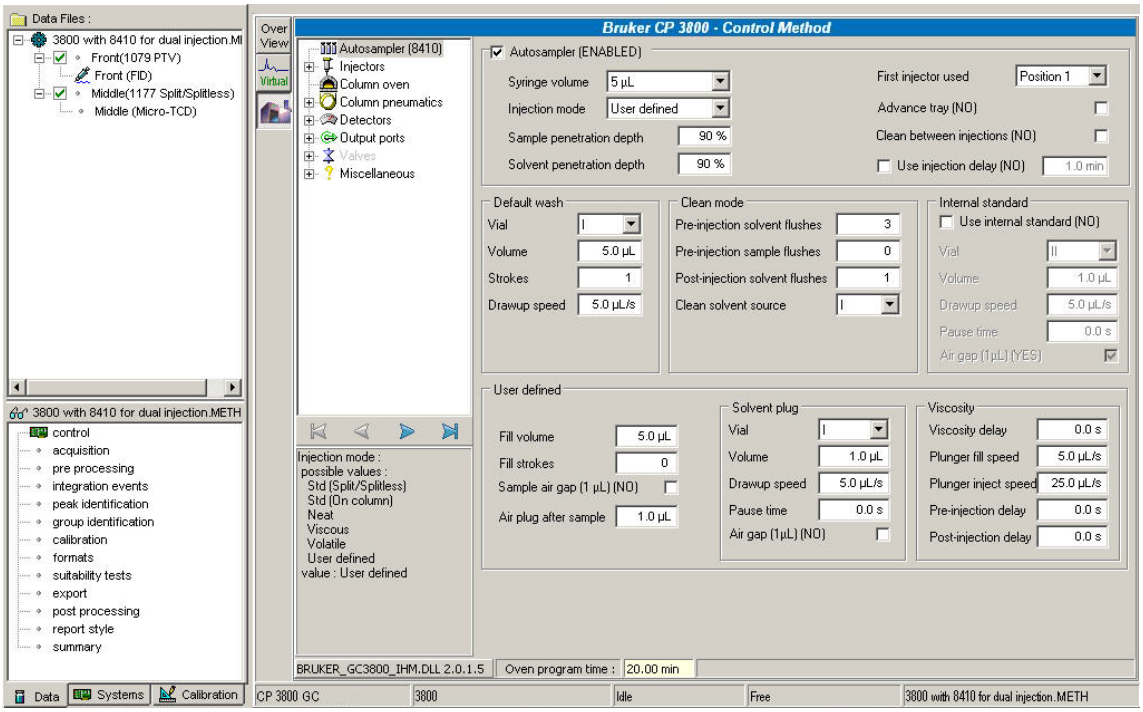


After Setup is uploaded successfully, click on the *OK* button.

You will need to *Start* and *Stop* the instrument before closing the CompassCDS Configuration Manager or before proceeding to the CompassCDS software.

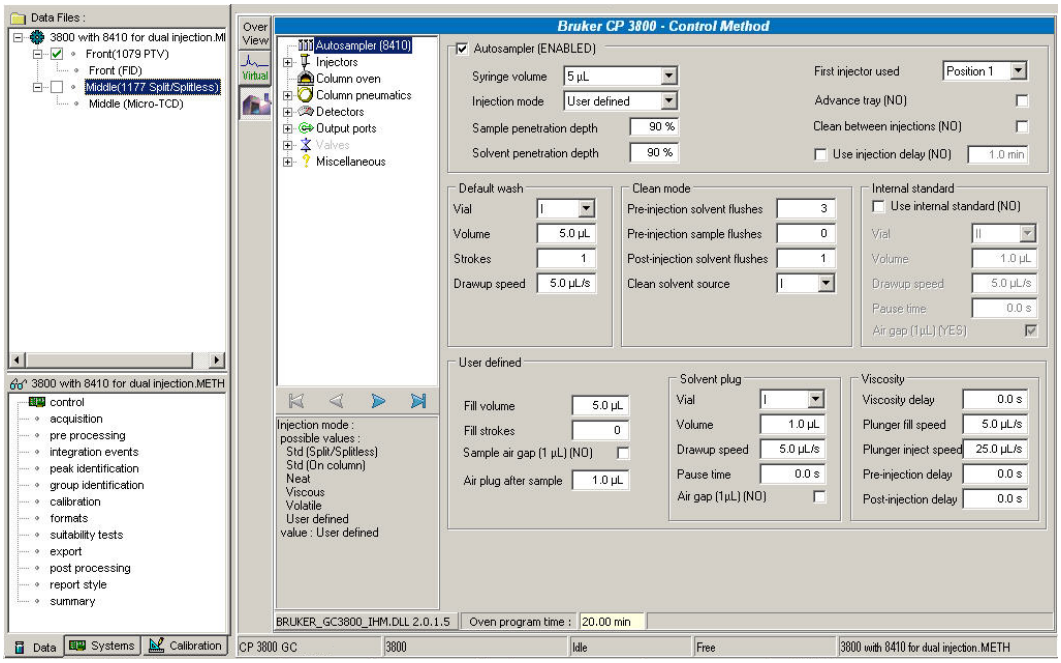
After successfully configuring the system in the CompassCDS Configuration Manager, open your instrument in CompassCDS and build a method for it by uploading the method from the instrument. Click on the *Data* tab at the bottom of the CompassCDS screen and display the method. Click on the *Autosampler* selection to show the Autosampler method. Your screen should look similar to the one displayed below. If you do not see selections for first injector used, Advance tray, etc., as

displayed in the upper right corner below, then the 3800 is not configured to use both injectors. Go back to the beginning of this document and verify that you have correctly set the 3800 to use both injectors.



Note the left side of the screen above. The expanded tree under the method shows two checkboxes for injectors Front (1079 PTV) and Middle (1177 Split/Splitless). Use these checkboxes to identify which of the two injectors you wish to use in the case that injections into only one injector are required (refer to the CompassCDS manual, *Create a Method* section for details about the way to use mutli-injectors and/or multi-detectors systems).

In the example below the middle injector has been deselected. In this configuration injections will only be made into the front injector.



Refer to the following tables for details about each autosampler parameter.

Parameter	Description
Autosampler	When unchecked, this option allows manual injection and to not use the autosampler (when unchecked, all the autosampler parameters become non-active).
Syringe Volume (µL)	Selects the size of the syringe that is installed on the instrument.
Injection Mode	Consists of five predefined injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile. A sixth User Defined mode is available allowing access to all autosampler parameters to fine-tune the injection.
Sample Penetration Depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Penetration Depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
First Injector Used	Corresponds to the injector used for sample injection. If the autosampler is physically mounted in the Front position, position 1 will correspond to the front injector and position 2 will correspond to the middle injector. If the autosampler is physically mounted in the Rear position, position 1 will correspond to the middle injector and position 2 will correspond to the rear injector.
Advance Tray	When checked, this option allows injection from two successive vials in the two injectors (Dual Injection mode). When unchecked, the autosampler will inject from the same vial in the two injectors (Duplicate Injection mode).
Clean Between Injection	When checked, the sampler will perform a wash program before the injection from the second vial.
Use Injection Delay	Check this option to define a time delay before the injection from the second vial (note: between two injections, without setting an injection delay, the autosampler takes about 0.7 minutes).

NOTE:

- The standard mode is the default and typically yields good results in most applications
- The volatile sampling mode is used for sampling solvents with high vapor pressures at room temperature
- The neat sampling mode is used for pure samples requiring minimum contamination with wash solvent (this mode does not use a solvent plug).
- The viscous sampling mode is used for samples with a higher viscosity than water.

NOTE: Enter the same number of vials for each injector (Vial field in the Acquisition method section).

Default Wash Parameter Group

In the Default wash fields, define the parameters that will be used during the default cleaning, which is used in the case that automation is stopped or a serious fault is detected.

Parameter	Description
Vial	Specifies which of the three solvent vials will be used by the default cleaning.
Volume (µL)	Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Drawup Speed (µL/s)	Specifies speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

Clean Mode Parameter Group

In the Clean mode fields, define the pre-injection and post-injection syringe clean modes.

Parameter	Description
Pre-injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample, before injection.
Pre-injection Sample Flushes	Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.
Post-injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified), after injection.
Clean Solvent Source	Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.

Internal Standard Parameter Group

This parameter group is displayed when one of the following injection modes is selected: Viscous, Volatile, or User-defined.

If the Use internal standard option is checked, an internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.

Parameter	Description
Vial	Selects which solvent vial contains the internal standard.
Volume (µL)	Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup Speed (µL/s)	Specifies the speed at which the internal standard will be drawn up into the syringe.
Pause Time	Defines how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air Gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap between the internal standard and the sample

NOTE: When this mode of injection is selected, beware that the total volume (volume of sample injected, entered in the Volume field of the Acquisition method section + Volume of internal standard + volume of any air gaps) doesn't exceed the maximum syringe volume or the autosampler will be faulted and the GC will stay in the Waiting for injection state.

User Defined Parameter Group

When the User defined injection mode has been selected, another parameter group is displayed and allows you to define the general, solvent plug, and viscosity parameters:

User Defined Parameters

Parameter	Description
Fill Volume (µL)	Specifies the sample volume that will be used for each fill stroke.
Fill Strokes	Specifies the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.
Sample Air Gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the sample plug.
Air Plug after Sample	Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

Solvent Plug Parameters

Parameter	Description
Vial	Selects which solvent vial to use for the solvent plug.
Volume (µL)	Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup Speed (µL/s)	Specifies the speed at which the solvent will be drawn up into the syringe.
Pause Time	Defines how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the solvent plug.

Viscosity Parameters

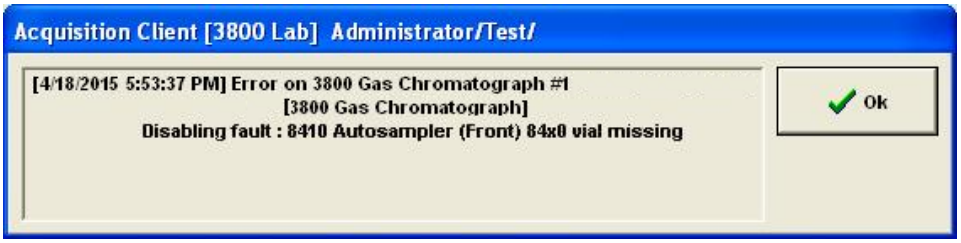
Parameter	Description
Viscosity Delay (sec)	Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Plunger Fill Speed (µL/sec)	Specifies the speed at which the sample will be drawn up into the syringe.
Plunger Inject Speed (µL/sec)	Specifies the speed at which the contents of the syringe will be expelled into the injector.
Pre-injection Delay (sec)	Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.
Post-injection Delay (sec)	Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

NOTE: When a vial is missing, the following message appears and you have 10 minutes to replace the sample in the correct vial position before the system skips the missing vial and passes to the next line of the sequence or stops the run. When you have replaced the missing sample, you must go to the Systems tab, click on the instrument icon, select the Miscellaneous window and click on the

button to restart the run.

If you want to skip the missing vial and start the next run, you must press the

button.


Acquisition Client [3800 Lab] Administrator/Test/
[4/18/2015 5:53:37 PM] Error on 3800 Gas Chromatograph #1
[3800 Gas Chromatograph]
Disabling fault : 8410 Autosampler (Front) 84x0 vial missing
Ok

Warning Message When a Vial is missing

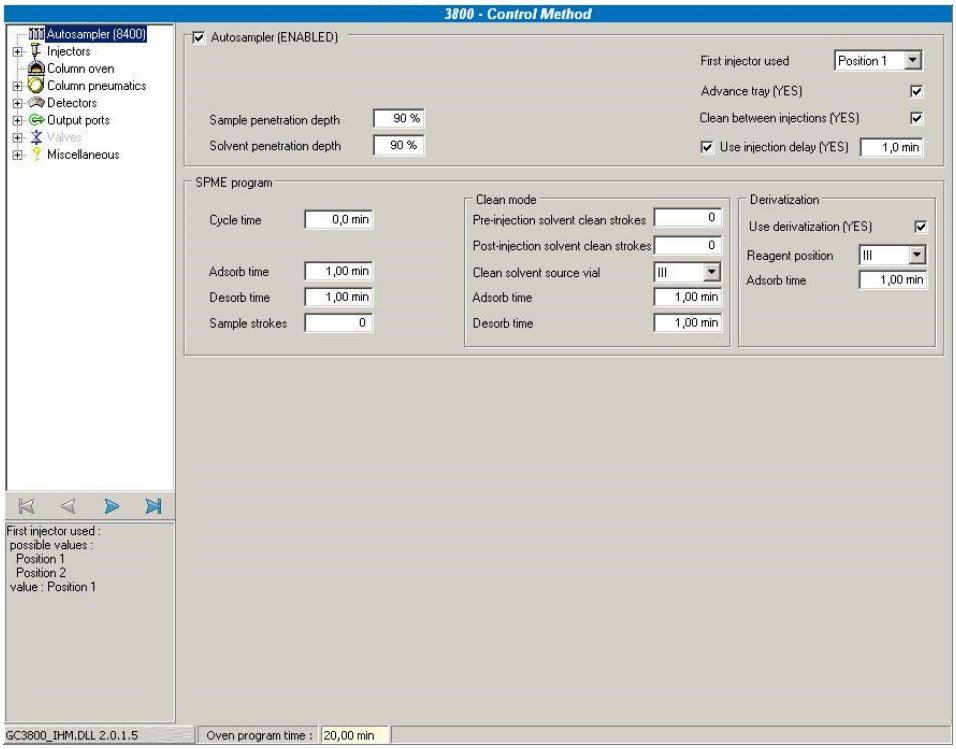
Default Settings for Predefined Autosampler Mode

The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

Parameter	Std Split/ Splitless	Std On-Column	Neat [1]	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, you must use User Defined mode.				
PreDefined Settings:					
Fill Volume	7.5 µL	7.5 µL	Not used	Not used	Not used
Fill Strokes	5	5	0 [1]	0	0
Sample Air Gap	No	No	No	No	No
Air Plug after Sample	1 µL	1 µL	1 µL	1 µL	1 µL
Viscosity Settings:					
Viscosity Delay	0 sec	0 sec	0 sec	6 sec	9.9 sec
Plunger Fill Speed	2 µL/sec	2 µL/sec	2 µL/sec	1 µL/sec	1 µL/sec
Plunger Inject Speed	50 µL/sec	2 µL/sec	50 µL/sec	1 µL/sec	5 µL/sec
Pre-Injection Delay	0 sec	0 sec	0 sec	0 sec	0 sec
Post-Injection Delay	0 sec	6 sec	0 sec	0 sec	12 sec

[1] Instead of fill strokes, Neat mode fills the syringe with sample at 2 µL/sec then expels it into the waste cup at 50 µL/sec a total of six times. Then it fills the syringe with sample at 2 µL/sec and expels it back into the sample vial at 50 µL/sec. This “pumping” action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.

SPME Mode



Refer to the following tables for details about each autosampler parameter.

Parameter	Description
Autosampler	When unchecked, this option allows you to inject manually and to not use the autosampler (when unchecked, all the sampler parameters become non-active).
Sample Penetration Depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Penetration Depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
First Injector Used	Corresponds to the injector used for sample injection. If the autosampler is physically mounted in the Front position, position 1 will correspond to the front injector and position 2 will correspond to the middle injector. If the autosampler is physically mounted in the Rear position, position 1 will correspond to the middle injector and position 2 will correspond to the rear injector.
Advance Tray	When checked, this option allows injection from two successive vials in the two injectors (Dual Injection mode). When unchecked, the autosampler will inject from the same vial in the two injectors (Duplicate Injection mode).
Clean Between Injection	When checked, the autosampler will perform a wash program before the injection from the second vial.
Use Injection Delay	Check this option to define a time delay before the injection from the second vial (Note: between two injections, without setting an injection delay, the autosampler takes about 0.7 minutes).

NOTE: Enter the same number of vials for each injector (Vial field in the Acquisition method section).

SPME Program Parameter Group

In the SPME Program fields, define the parameters that will be used during the SPME injections.

Parameter	Description
Cycle Time	Specifies the total time of an analysis. This parameter is required only if prep-ahead is used. When using prep-ahead, the prep-vial parameter in the sequence should be set to 2 for this driver.
Adsorb Time	Specifies the time the fiber will stay in the vial.
Desorb Time	Specifies the time the fiber will be exposed in the injector to desorb the sample.
Sample Stroke	Specifies how many times the adsorb time will be repeated before injection.

Clean Mode Parameters

Parameter	Description
Pre-injection Solvent Clean Strokes	Specifies the number of time the fiber will be cleaned before the injection.
Post-injection Solvent Clean Strokes	Specifies the number of times the fiber will be cleaned after the injection.
Clean Solvent Source Vial	Specifies the clean solvent source vial.
Adsorb Time	Specifies the time the fiber will stay in the clean solvent source vial.
Desorb Time	Specifies the desorb time during the cleaning cycle.

Derivatization Parameters

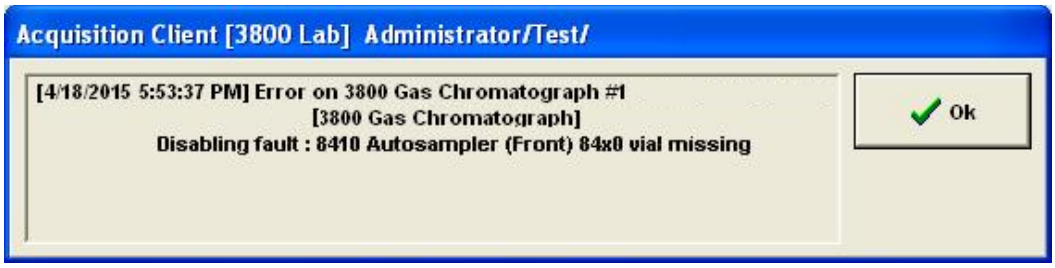
Parameter	Description
Use Derivatization	Specifies if derivatization will be used.
Reagent Position	Specifies the reagent vial.
Adsorb time	Specifies the time the fiber will stay in the reagent vial.

NOTE: When a vial is missing, the following message appears. You have 10 minutes to replace the sample in the correct vial position before the system skips the missing vial and passes to the next line of the sequence or stops the run. When you have replaced the missing sample, you must go to the *Systems* tab, click on the instrument icon, select the *MISCELLANEOUS* window and click on the

button to restart the run.

If you want to skip the missing vial and start the next run, you must press the

button.


Acquisition Client [3800 Lab] Administrator/Test/
[4/18/2015 5:53:37 PM] Error on 3800 Gas Chromatograph #1
[3800 Gas Chromatograph]
Disabling fault : 8410 Autosampler (Front) 84x0 vial missing
Ok

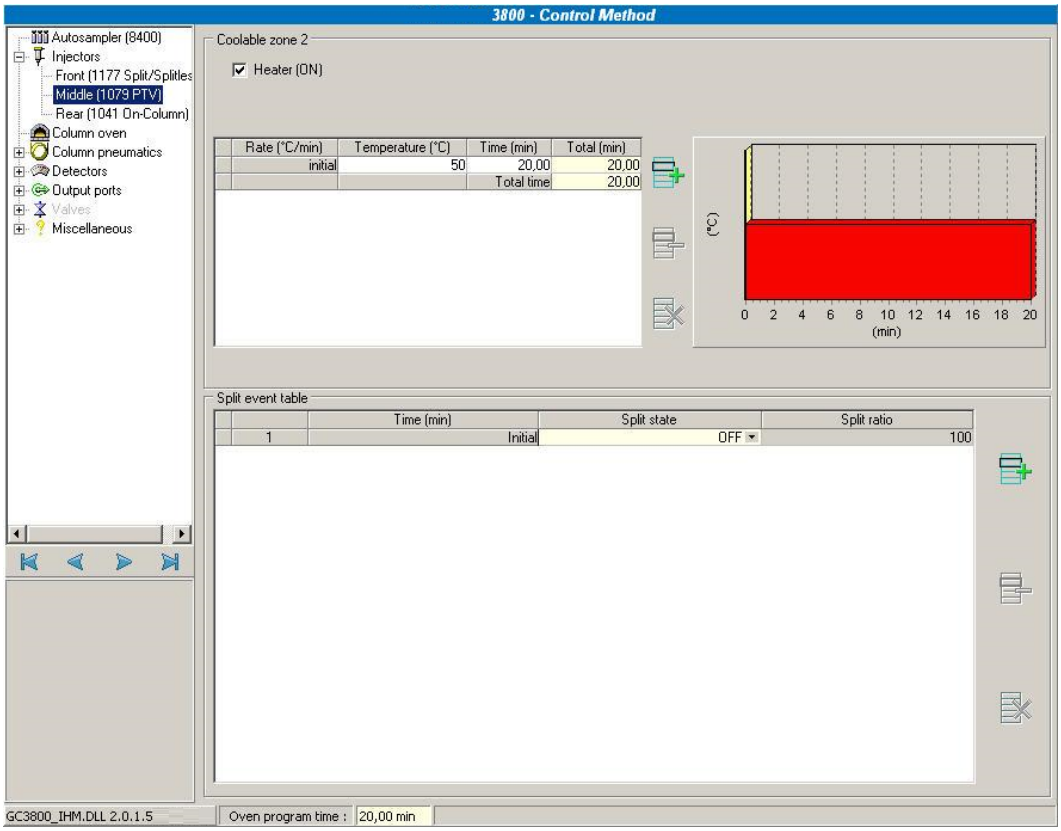
Warning Message When a Vial is missing

Injectors Control

The Injectors sub-section contains up to three injectors: Front, Middle, and Rear. Click on the injector you want to edit.

Depending on the system configuration, an injector can be connected to a heat-only zone or to a coolable zone with the coolant activated or not. In these cases, the screens displayed are not exactly the same.

1079 Injector



Coolable Zone or Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to indicate whether or not you will use the installed injector.

If the injector is connected to a coolable zone and if the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the injector. The first row of the table contains the initial temperature and hold time for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate* (°C/min) and the *Time* the inlet heater is held at this temperature in the corresponding columns.

NOTE: The graph shows the inlet temperature programming.

Split Event Table Parameter Group

If the injector is connected to a Type 1 EFC, you can build a split ratio time program by using the split event table.

The first row of the table contains the *Initial Split state* and *Split ratio* for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed.

The remainder of the table contains the time-programmed settings for the injector *Split ratio.* The split valve will be switched to the ratio in each row at the indicated time. If the *Split state* is ON, then the sample is split according to the split ratio specified in the corresponding column. If the state is OFF, the entire sample enters the column. The split ratio is defined as the column flow plus the split flow, divided by the column flow.

NOTE:

- You must have already configured the Type 1 EFC in the CompassCDS Configuration Manager before you can program the split ratio. Specifically, to build a 1079 Split Ratio Program, a Front 1079 must have a corresponding Front Type 1 EFC, a Middle 1079 must have a corresponding Middle Type 1 EFC, and a Rear 1079 must have a corresponding Rear Type 1 EFC.
- You can use a split ratio of 100 after injection to vent the injector of any residual solvent.
- Use a very low split ratio after flushing to conserve carrier gas.

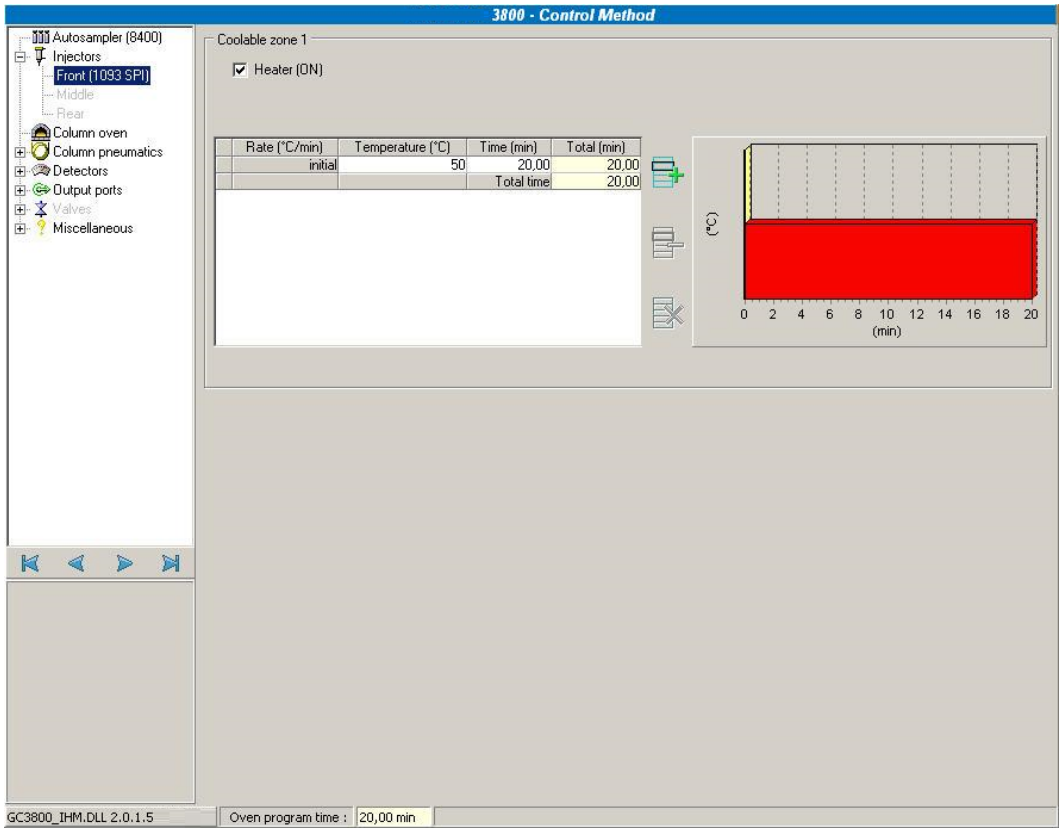
Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

1093 Injector



Coolable Zone Parameter Group

Check or uncheck the *Heater* option to indicate whether or not you will use the installed injector.

If the injector is connected to a coolable zone and if the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the injector. The first row of the table contains the initial temperature and hold time for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate* (°C/min) and the *Time* the inlet heater is held at this temperature in the corresponding columns.

NOTE: The graph shows the inlet temperature programming.

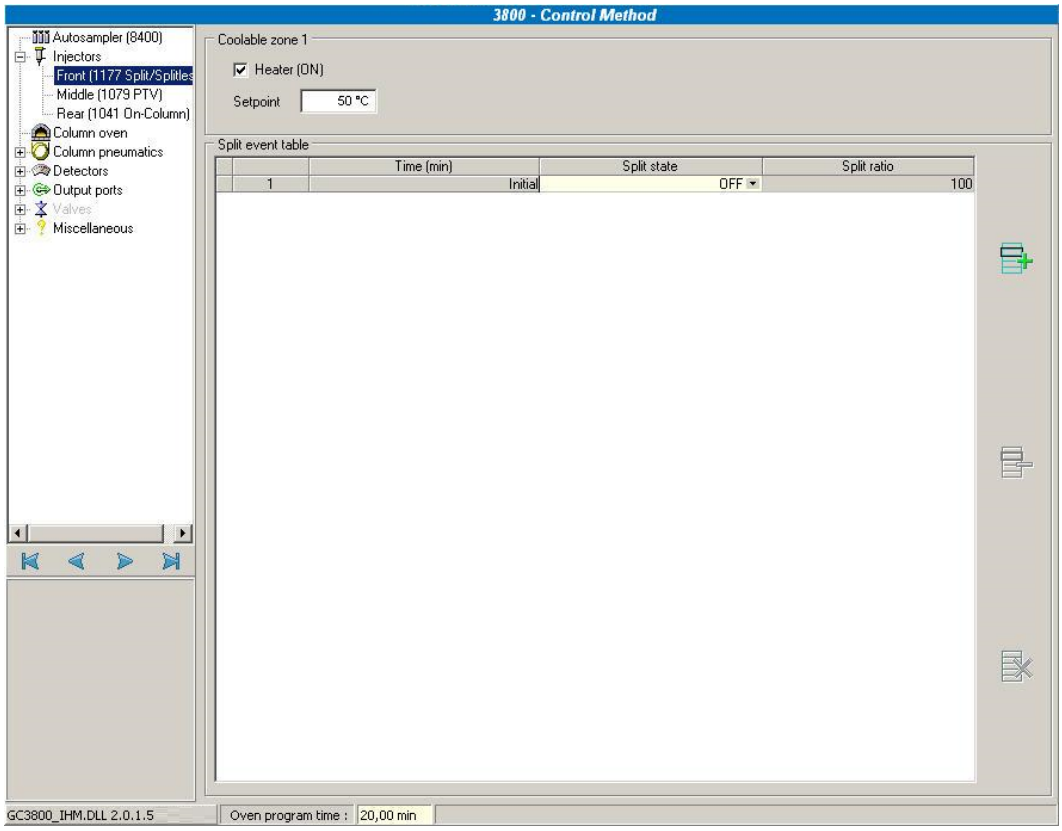
Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

1177 Injector



Coolable Zone or Heat-only Zone Parameter Group

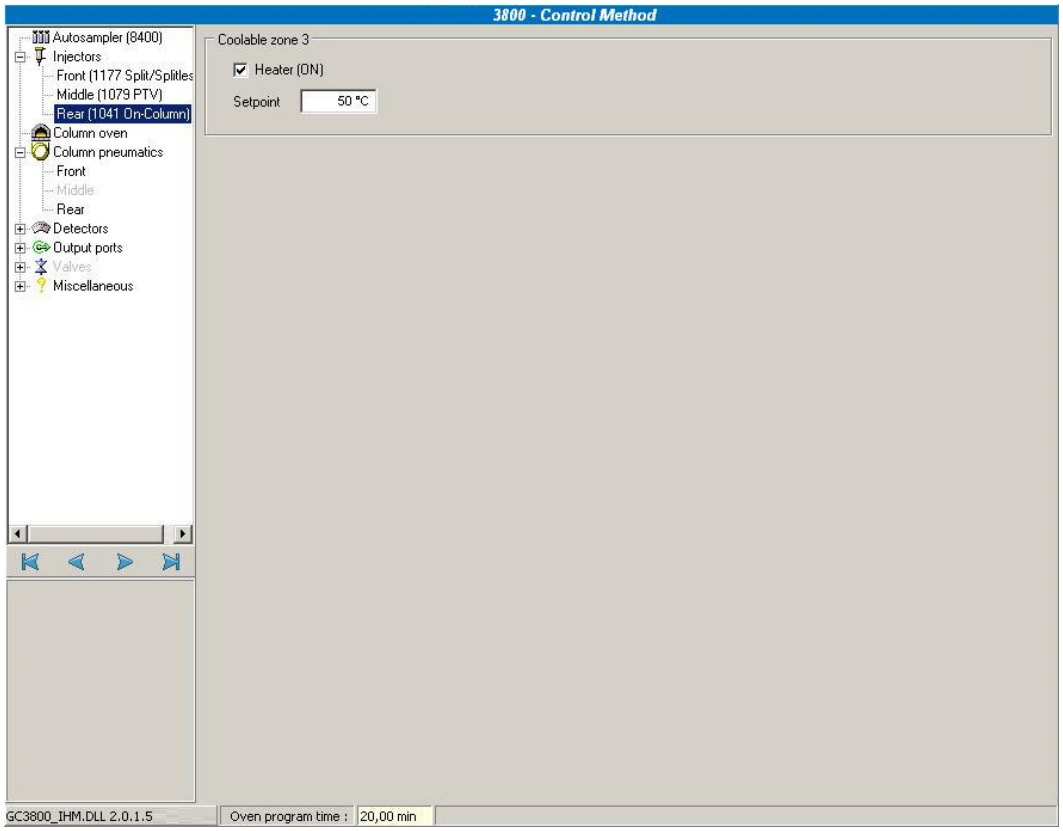
Check or uncheck the *Heater* option to turn the injector oven ON or OFFON or OFF.

Enter the injector oven temperature in the *Setpoint* field.

Split Event Table Parameter Group

If the injector is connected to a Type 1 EFC, you can build a split ratio time program by using the split event table (refer to the 1079 injector for more details).

1041 injector / 1061 injector

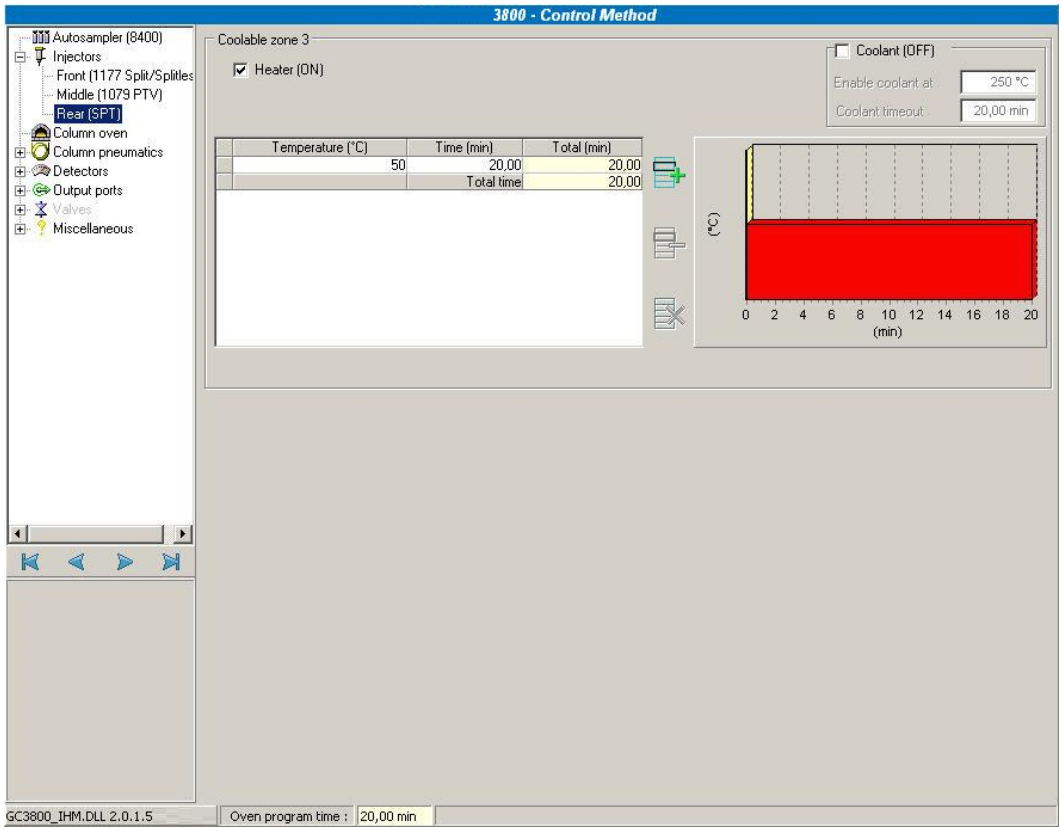


Coolable zone or Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the injector oven ON or OFFON or OFF.

Enter the injector oven temperature in the *Setpoint* field.

SPT injector (Sample Preconcentration Trap)



Coolable Zone Parameter Group

Check or uncheck the *Heater* option to turn the injector oven ON or OFFON or OFF.

The SPT must be connected to coolable zone 3. If the coolant is activated, check the *Coolant* option if you want to turn the coolant valve ON when the injector is cooling down. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the injector fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature program to heat and/or cool the injector.

Enter the final temperature of each segment in the *Step* column and the *Time* the inlet heater is held at this temperature in the corresponding column.

Use the following buttons to edit the table:

To add a line to the table.

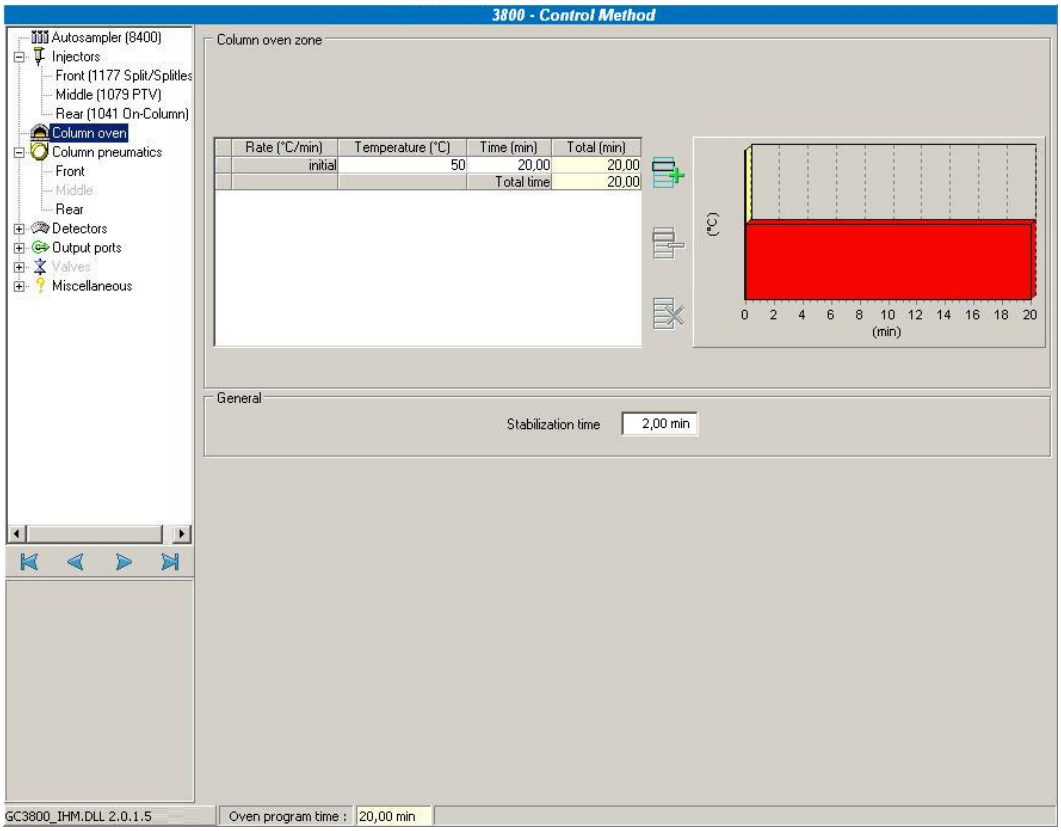
To delete a line in the table.

To clear the entire table.

NOTE: The graph shows the inlet temperature program.

Column Oven Control

The Column oven window contains the column oven program:



Column Oven Zone Parameter Group

Check the *Coolant* option if you want to turn the column coolant valve ON. Specify the temperature (°C) for the coolant valve to turn on in the *Enable coolant at* field and the *Coolant timeout*. This parameter provides a safety measure to save coolant after the specified time if the column oven fails to reach its set temperature or the GC does not go into run mode. The valve will be turned OFF if the coolant timeout is reached and no further coolant will be applied.

Use the table to build a temperature ramp program to heat and/or cool the column oven.

The first row of the table contains the Initial temperature and Hold time for the column oven. The column oven will equilibrate to this setting and stabilize for the specified *Stabilization time* (defined in the General parameter group), when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the *Step* column, the *Rate* (°C/min) and the *Time* the column oven is held at this temperature in the corresponding columns.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

NOTE: The graph shows the column oven temperature program.

General Parameter Group

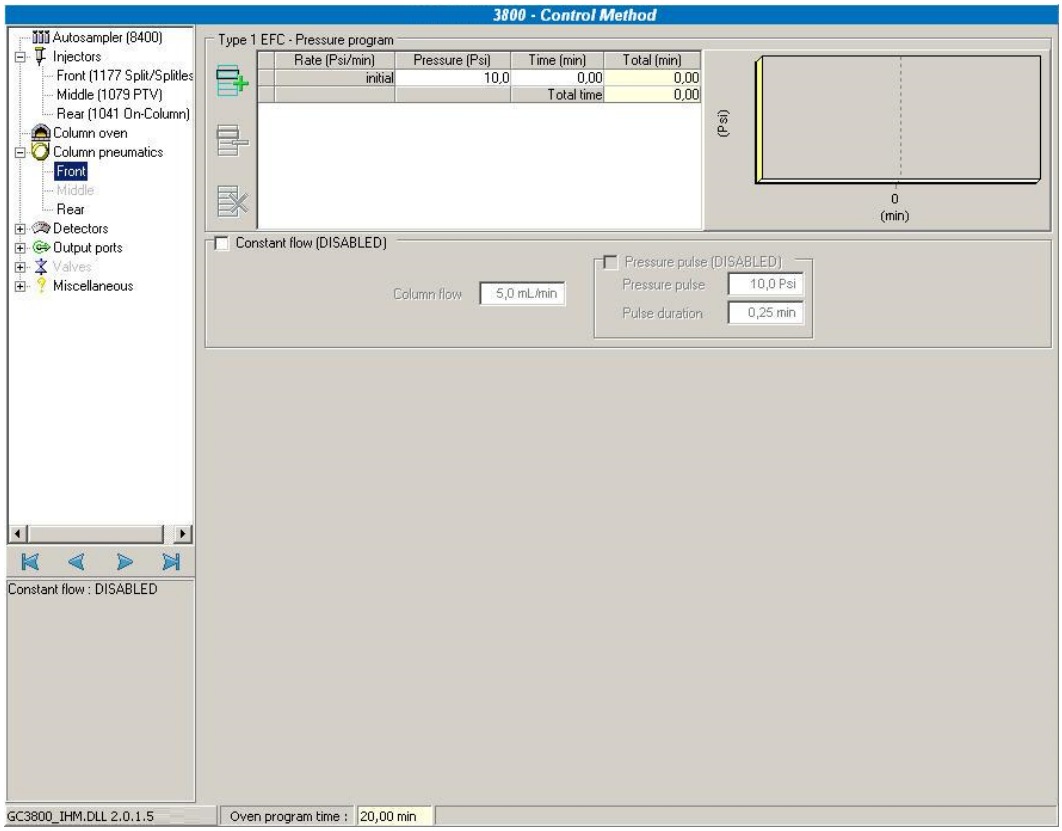
Enter the *Stabilization time* in the corresponding field.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Column Pneumatics Control

The Column pneumatics window contains up to three Electronic Flow Control (EFC) Programs (Front, Middle, Rear). Use the EFC Programs to specify the pressure ramp of the Type 1, Type 2 and Type 5 EFC, the pressure ramp and total flow time program of the Type 4 EFC, and the flow ramp of the Type 3 EFC.

Type 1 EFC (for 1079/1177 split/splitless injectors)



NOTE: Type 1 and Type 5 EFCs are identical except with respect to the mechanical plumbing of the pressure sense line. Type 5 EFCs are identified as Type 1 EFCs in software.

Pressure Program Parameter Group

Use the table to build a pressure ramp program.

The first row of the table contains the initial pressure and hold time for the Type 1 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate* (psi/min) and the *Time* the EPC is held at this pressure in the corresponding columns.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

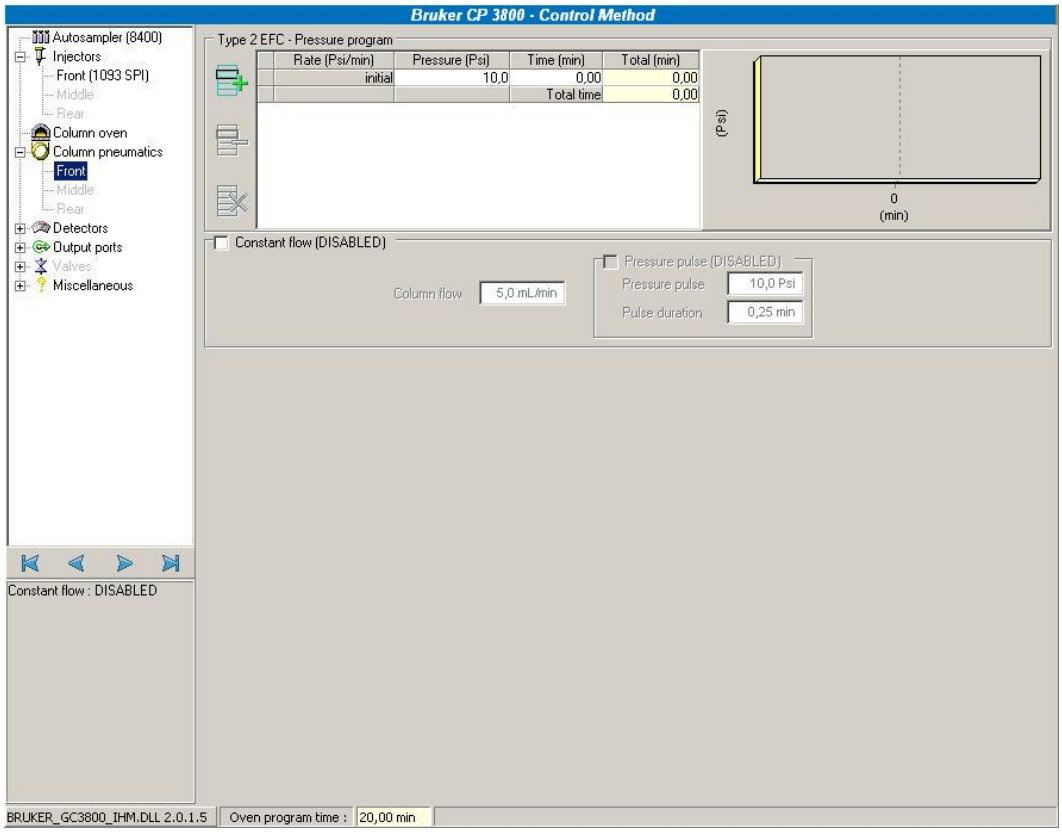
NOTE: The graph shows the pressure ramp program.

Constant flow Parameter Group

Check the *Constant flow* option to disable the table and enter the desired constant *Column flow* (mL/min) in the corresponding field.

Check the *Pressure pulse* option to perform a pressure pulse injection. Prior to injection, the pressure will change to the *Pressure pulse* pressure. After injection, the Pressure pulse pressure will be maintained for the *Pulse duration*.

Type 2 EFC (for 1093 injector)



Pressure Program Parameter Group

Use the table to build a pressure ramp program.

The first row of the table contains the initial pressure and hold time for the Type 2 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate* (psi/min) and the *Time* the EPC is held at this pressure in the corresponding columns.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

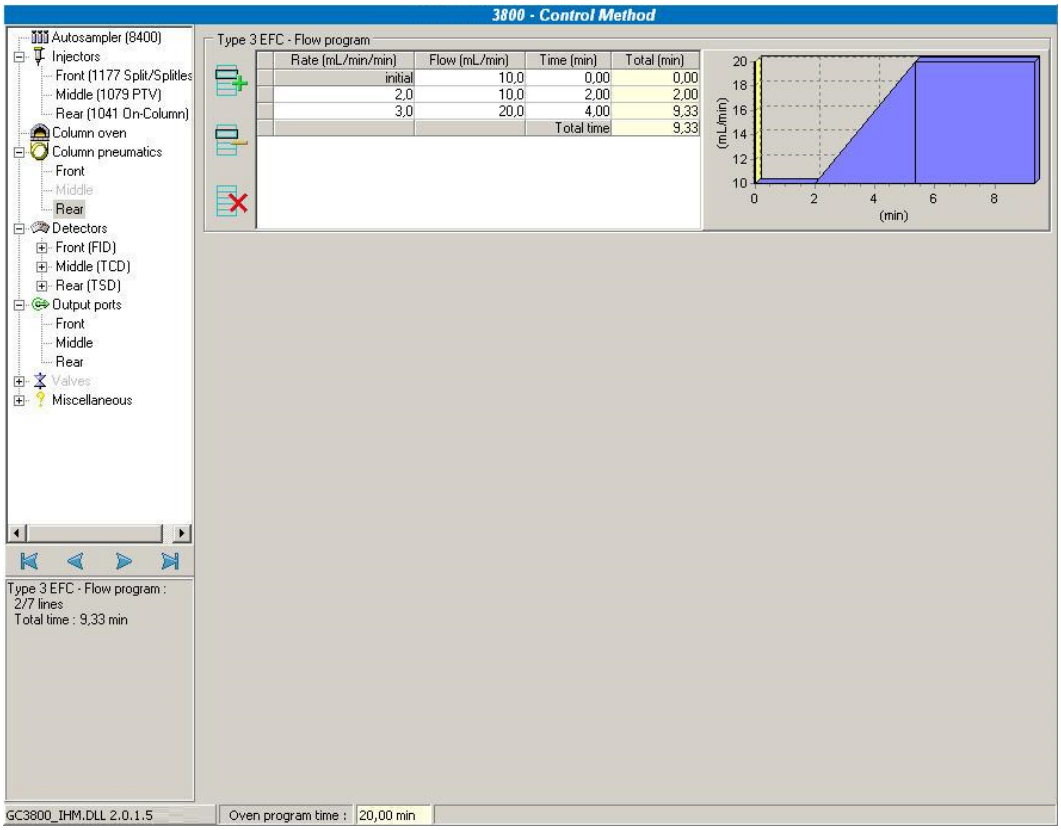
NOTE: The graph shows the pressure ramp program.

Constant Flow Parameter Group

Check the *Constant flow* option to disable the spreadsheet and enter the desired constant *Column flow* (mL/min) in the corresponding field.

Check the *Pressure pulse* option to perform a pressure pulse injection. Prior to injection, the pressure will change to the *Pressure pulse* pressure. After injection, the Pressure pulse pressure will be maintained for the *Pulse duration*.

Type 3 EFC (for packed columns)



Flow Program Parameter Group

Use the table to build a flow ramp program.

The first row of the table contains the initial flow and hold time for the Type 3 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final flow of each ramp segment in the *Flow* column, the *Rate* (mL/min/min) and the *Time* the segment is held at this flow in the corresponding columns.

Use the following buttons to edit the table:

To add a line to the table.

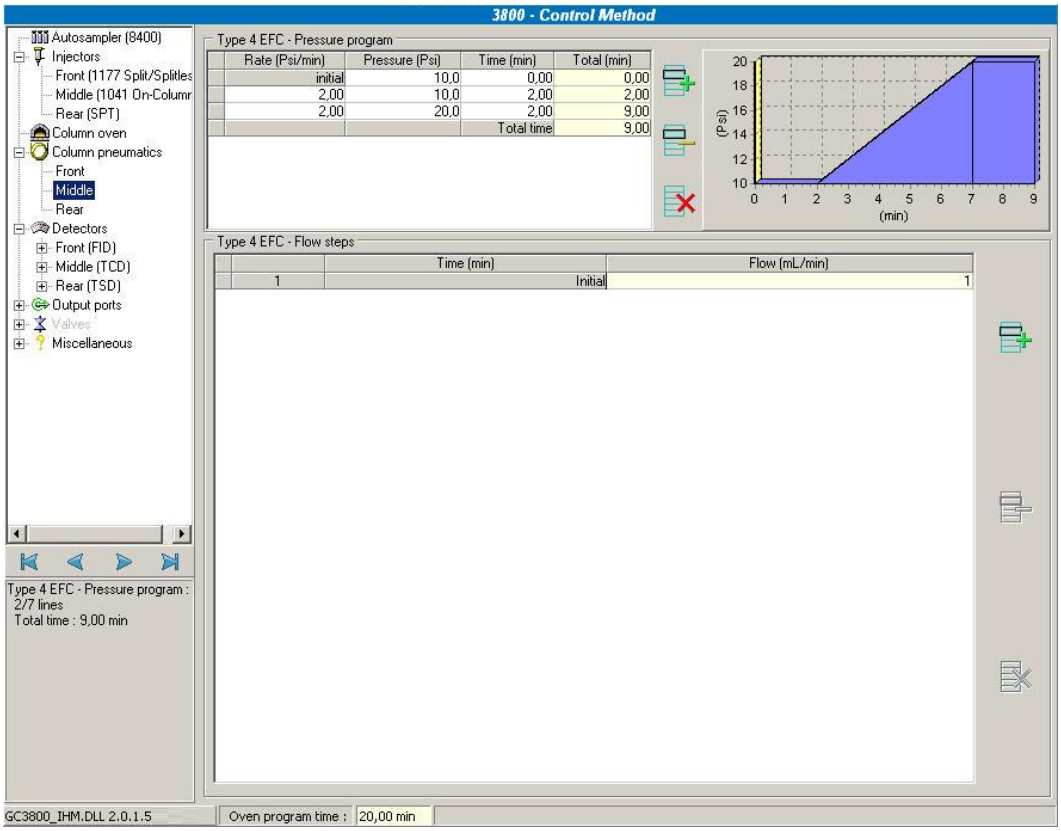
To delete a line in the table.

To clear the entire table.

NOTE: The graph shows the flow ramp program.

Type 4 EFC (for 1041/1061 and valved systems)

If a Type 4 EFC is installed, a pressure ramp table and a flow time program table will appear:



Pressure Program Parameter Group:

Use the first table to build a pressure ramp program.

The first row of the table contains the initial pressure and hold time for the Type 4 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the *Pressure* column, the *Rate* (psi/min) and the *Time* the EPC is held at this pressure in the corresponding columns.

NOTE: The graph shows the pressure ramp program.

Flow Steps Parameter Group:

Use the second table to build a flow time program to control the Type 4 EFC total flow.

The first row of the flow table contains the initial total flow for the Type 4 EFC.

The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The remainder of the table contains the time-programmed settings for the total flow. The total *Flow* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

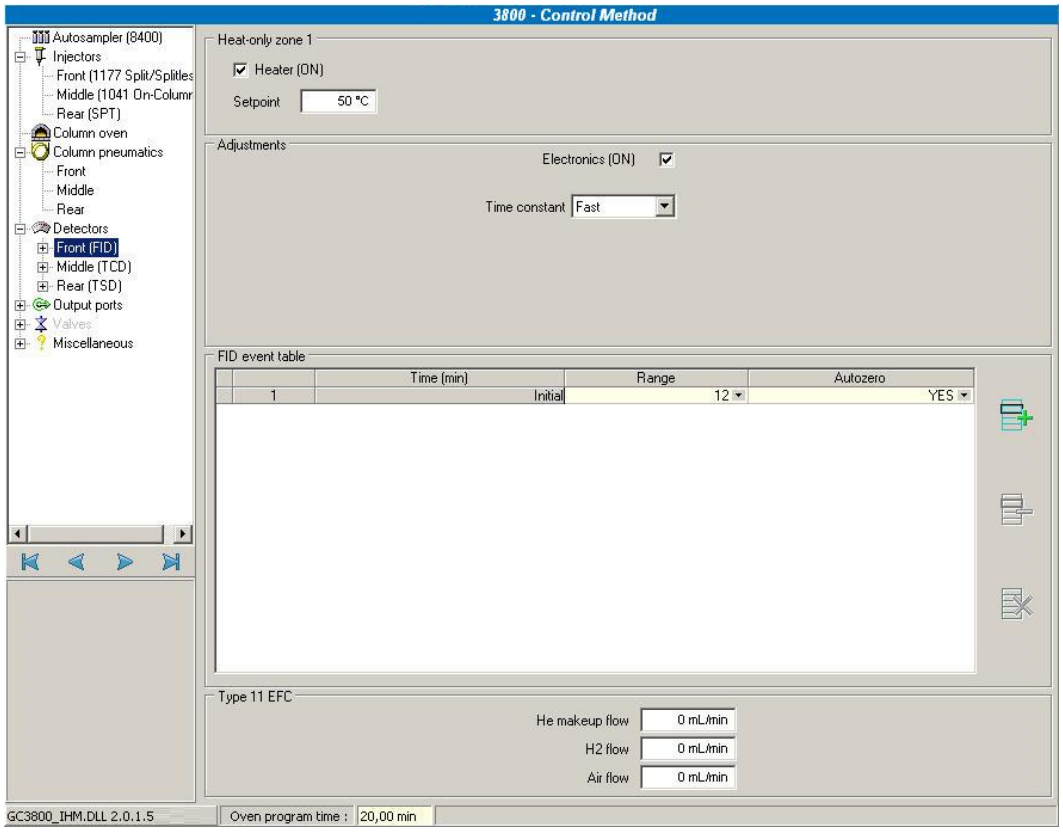
To delete a line in the table.

To clear the entire table.

Detectors Control

The Detectors sub-section contains up to three detectors: Front, Middle, and Rear. Click on the detector you want to edit and specify the operating temperatures, gas flow rates, and specific parameters:

FID Detector (Flame Ionization Detector)



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the detector oven ON or OFFON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments Parameter Group

Check or uncheck the *Electronics* option to indicate whether the installed FID will be used or not. Select the required *Time constant* from the list.

FID Event Table Parameter Group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range* and *Autozero* for the FID detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run starts.

The remainder of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

Type 11 EFC Parameter Group

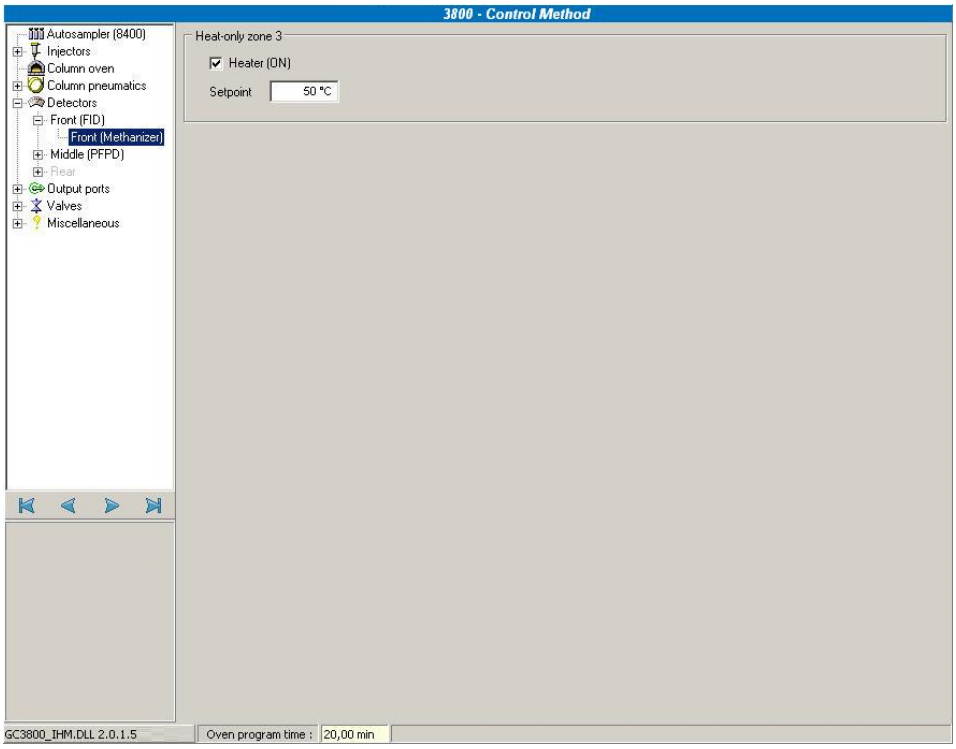
If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and allow you to define the desired gas flow rates.

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For FID detectors, the EFC Type 11 is required.

Methanizer

A methanizer is an option that converts carbon monoxide and carbon dioxide to methane.

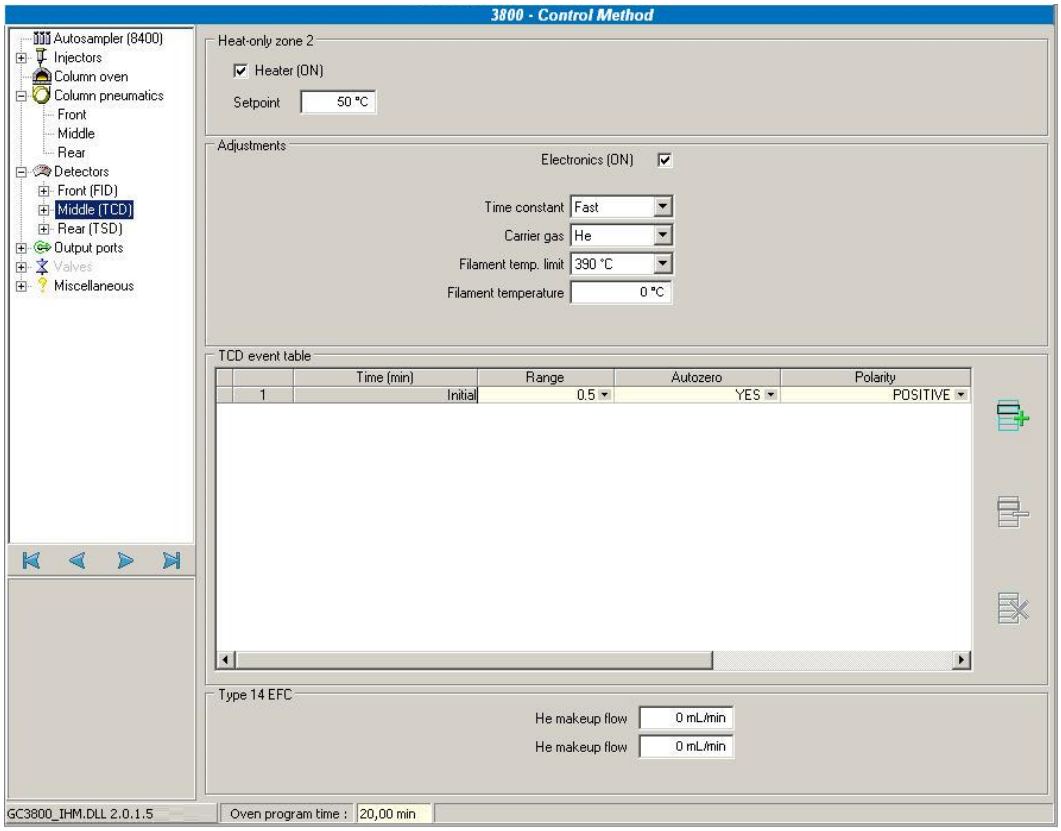
It is associated with a specific FID detector; consequently, it is accessed in the *Detector* section:



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the methanizer oven ON or OFF and enter the methanizer oven temperature in the *Setpoint* field.

TCD Detector (Thermal Conductivity Detector)



Heat-only zone Parameter Group

Check or uncheck the Heater option to turn the detector oven ON or OFF and enter the detector oven temperature in the Setpoint field.

Adjustments Parameter Group

Check or uncheck the *Electronics* option to indicate whether the installed TCD will be used or not. Select the required *Time constant* from the list.

Choose the *Carrier gas*: If you are using helium or hydrogen as carrier gas, select the He setting. For all other carrier gases, select the N2/Ar setting.

Specify the *Filament temperature* in the corresponding field and select the *Filament temperature limit* from the list. To protect the filament, always operate the detector with the 390 °C limit selected unless you require the maximum dynamic range available to the TCD. With the limit set to 390°C, the peak sample filament temperature is limited to approximately 450 °C. The temperature limit is approximately 550°C at the 490°C setting. The 450°C limit protects filaments from oxidation when exposed to air over an extended period of time. However, at the 550 °C temperature limit the filament can degrade after only a few minutes.

TCD Event Table Parameter Group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range*, *Autozero* and *Polarity* for the TCD detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run

starts. The polarity is used to reverse the peaks that appear in the negative direction (for example, if you inject a standard or sample into the reference side of the TCD).

The remainder of the table contains the time-programmed settings: the *Range*, *Autozero* and *Polarity* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

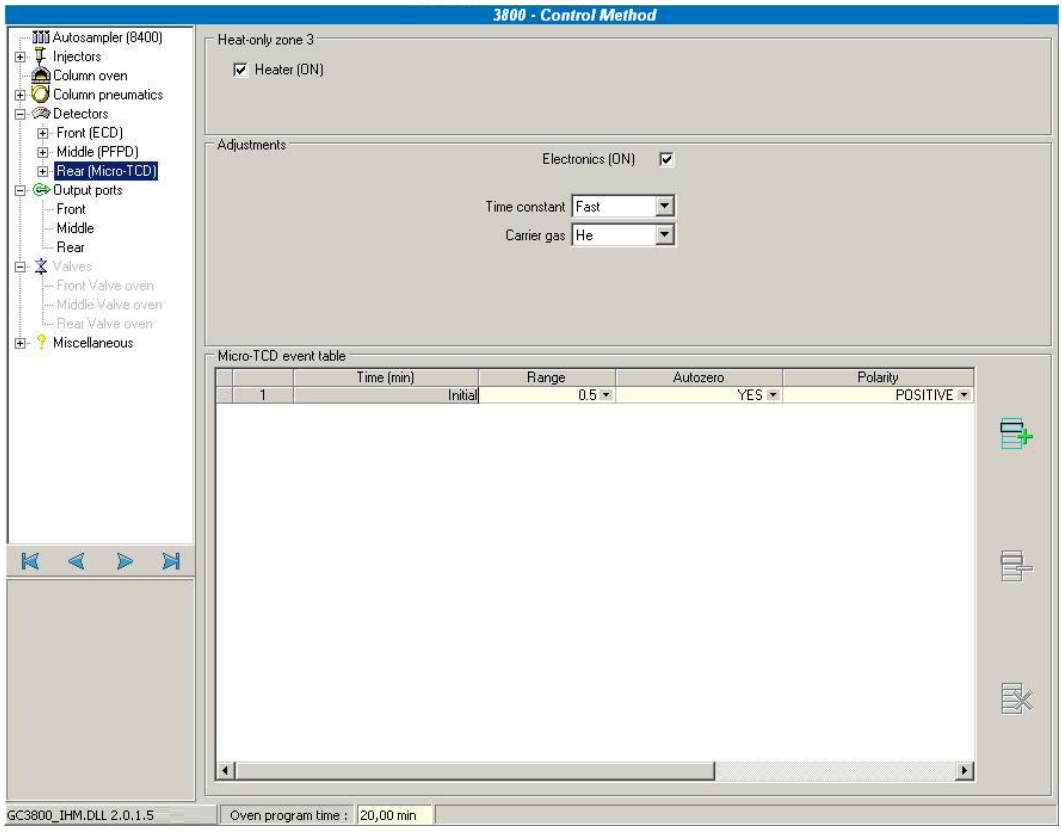
Type XY EFC Parameter Group

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For TCD detectors, three EFC types are available: Type 13, Type 14 and Type 16.

If the detector Electronic Flow Control module is installed, the Type XY EFC section will appear and allows you to define the desired gas make up flow rate.

Micro-TCD Detector

If a Micro-TCD Detector is installed, the following window will appear (refer to the TCD detector for details). The Micro-TCD event table enables you to time-program the detector range, autozero, and polarity.



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the detector oven ON or OFF.

NOTE: The Micro-TCD cell temperature is set to 110 °C and is not adjustable.

Adjustments Parameter Group

Check or uncheck the *Electronics* option to indicate whether the installed TCD will be used or not. Select the required *Time constant* from the list.

Choose the *Carrier gas*: If you are using helium or hydrogen as carrier gas, select the He setting. For all other carrier gases, select the N_2/Ar setting.

Micro-TCD Event Table Parameter Grou:

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range*, *Autozero* and *Polarity* for the TCD detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run starts. The polarity is used to reverse the peaks that appear in the negative direction (for example, if you inject a standard or sample into the reference side of the TCD).

The rest of the table contains the time-programmed settings. The *Range*, *Autozero* and *Polarity* will be switched to the value in each row at the indicated *Time*.

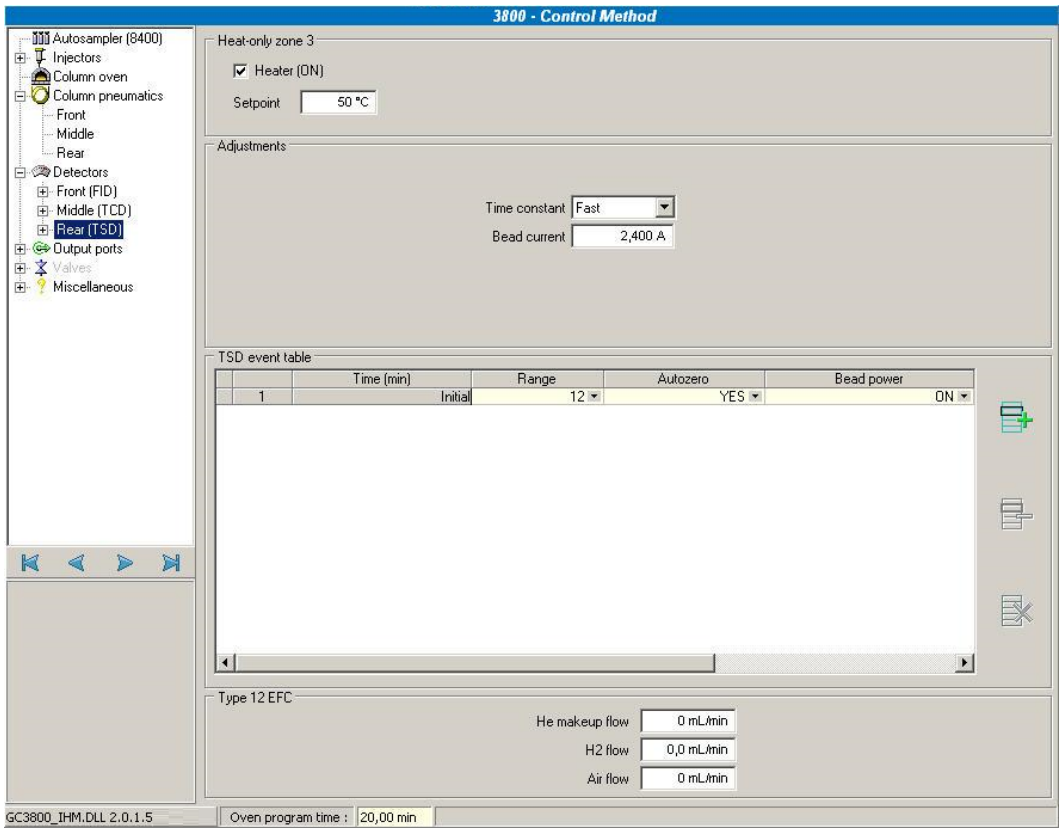
Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

TSD Detector (Thermionic Specific Detector)



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments Parameter Group

Select the required *Time constant* from the list.

Specify the *Bead current* (i.e., bead surface temperature) in the corresponding field; it corresponds to the current at which the gas phase chemistry will initiate.

TSD Event Table Parameter Group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range*, *Autozero* and *Bead power* state for the TSD detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run starts.

The remainder of the table contains the time-programmed settings: the *Range*, *Autozero* and *Bead power* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

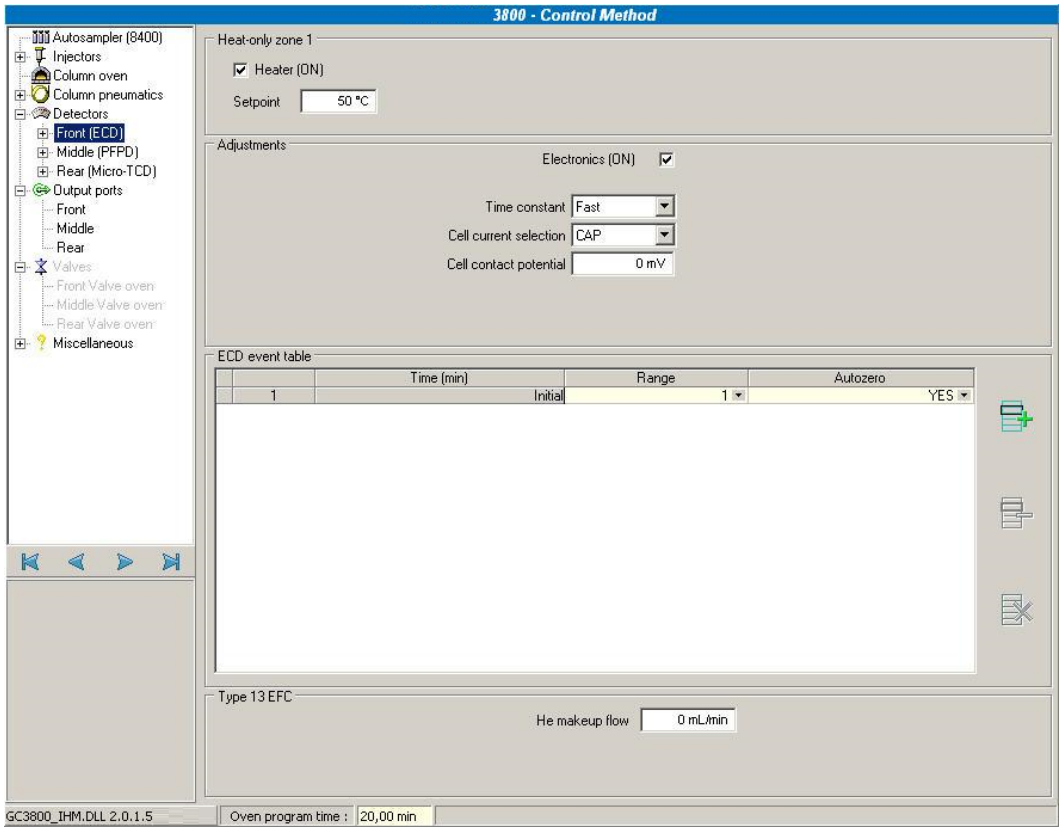
To clear the entire table.

Type 12 EFC Parameter Group

If the detector Electronic Flow Control module is installed, the Type 12 EFC section will appear and allows you to define the desired gas flow rates.

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the Configuration Manager. For TSD detectors, EFC Type 12 is required.

ECD Detector (Electron Capture Detector)



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments Parameter Group

Check or uncheck the *Electronics* option to indicate whether the installed ECD will be used or not.

Select the required *Time constant* from the list. For most applications, select the SLOW setting. For capillary applications with peak widths at half height of less than 2 seconds, select the FAST setting.

Specify the *Cell current* and *Cell contact potential* in the corresponding fields.

The choice of cell current depends on the specific carrier gas that is used and the baseline signal with only carrier gas present. For normal operation with nitrogen carrier gas, use the N2STD or CAP setting. When a greater linear range is desired, select the Ar/CH4 setting and use 90%Argon / 10% Methane as the carrier gas.

ECD Event Table Parameter Group

Use the table to change detector settings during the analysis.

The first row of the table contains the initial *Range* and *Autozero* for the ECD detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run starts.

The remainder of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

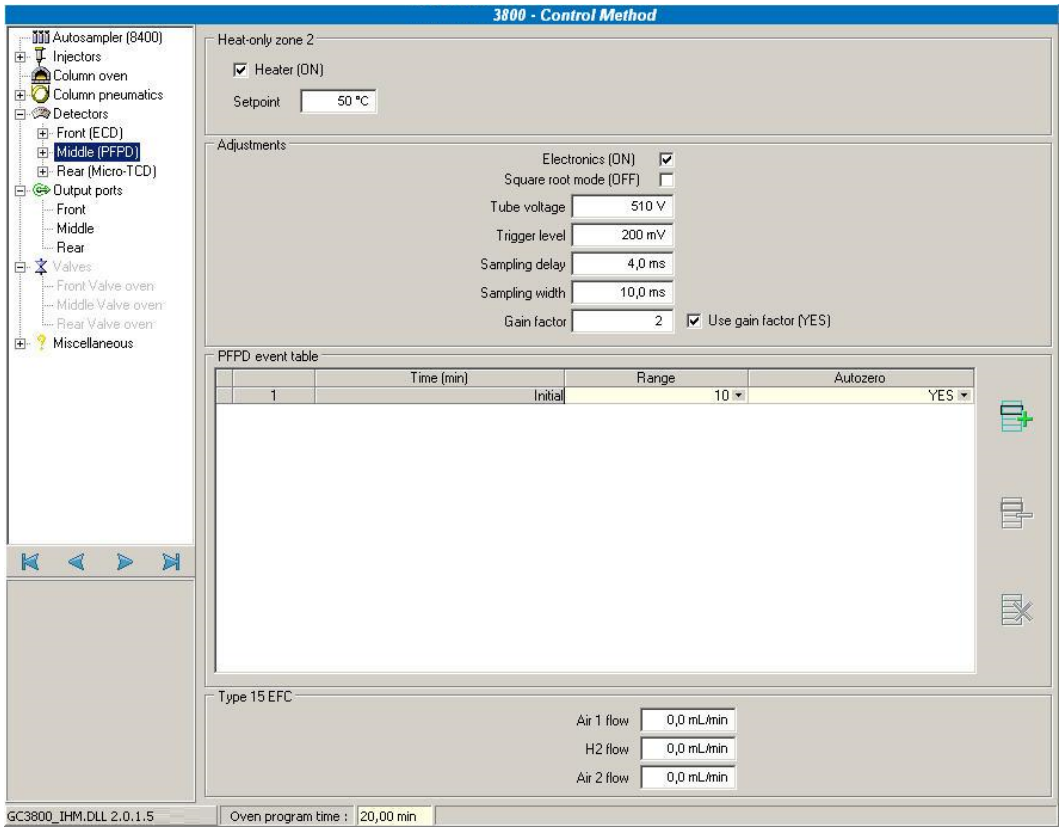
To clear the entire table.

Type 13 EFC Parameter Group

If the detector Electronic Flow Control module is installed, the Type 13 EFC section will appear and allows you to define the desired gas make-up flow rate.

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For ECD detectors, the EFC Type 13 is required.

PFPD Detector (Pulsed Flame Photometric Detector)



Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to turn the detector oven ON or OFF and enter the detector oven temperature in the *Setpoint* field.

Adjustments Parameter Group

Check or uncheck the *Electronics* option to indicate whether the installed PFPD will be used or not.

Check or uncheck the *Square root mode* option to enable or disable this mode.

Enter the PFPD photomultiplier voltage in the *Tube voltage* field and select the desired *Trigger level*, *Sampling delay, Sampling width,* and *Gain factor* in the corresponding fields.

PFPD event table Parameter Group

Use the table to change detector settings during the analysis.

The first row of the table contains the *initial Range* and *Autozero* for the PFPD detector. When the initial autozero is set to yes, the detector autozero is on continuously before the run starts.

The remainder of the table contains the time-programmed settings: the *Range* and *Autozero* will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

To add a line to the table.

To delete a line in the table.

To clear the entire table.

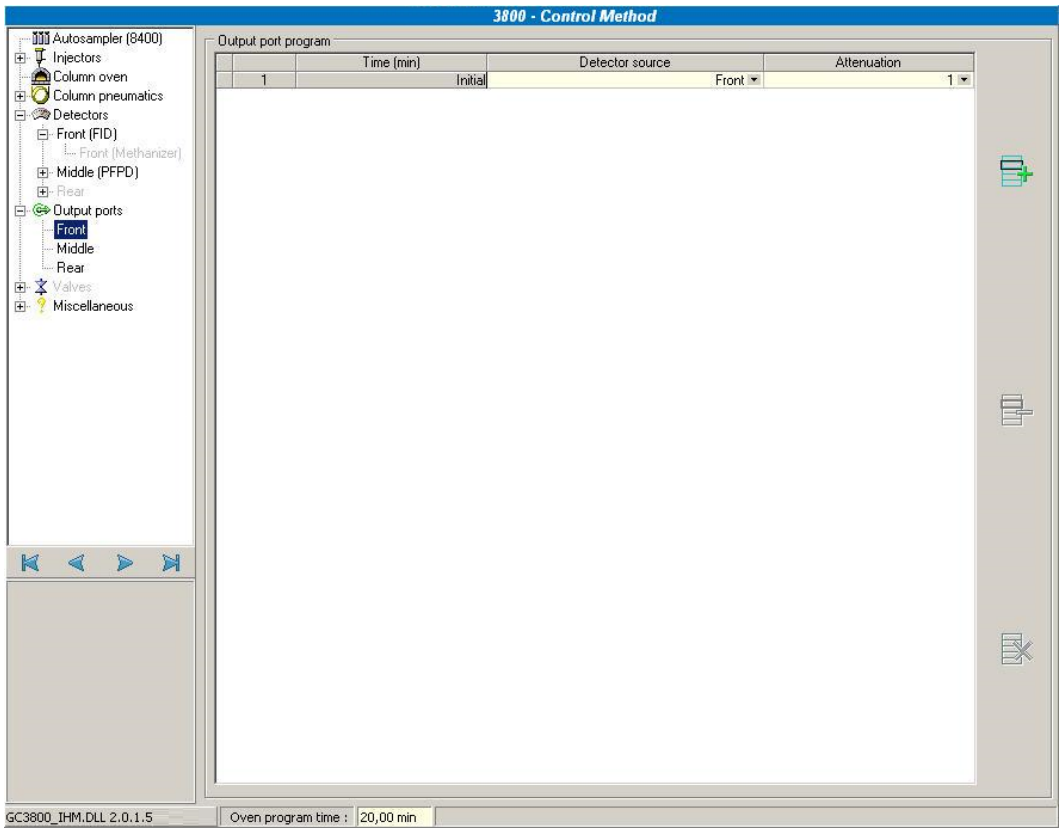
Type 15 EFC Parameter Group

If the detector Electronic Flow Control module is installed, the Type 15 EFC section will appear and allows you to define the desired gas flow rates.

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For PFPD detectors, the EFC Type 15 is required.

Output Ports Control

The 3800 GC has three analog output ports, which allow analog data to be sent to external integrators or other analog data systems:



Output Port Program Parameter Group

Use the table to time program the *Detector* signal *source* and *Attenuation* at each port. The first row of the table contains the initial signal *source* and *Attenuation* for the port.

Use the following buttons to edit the table:

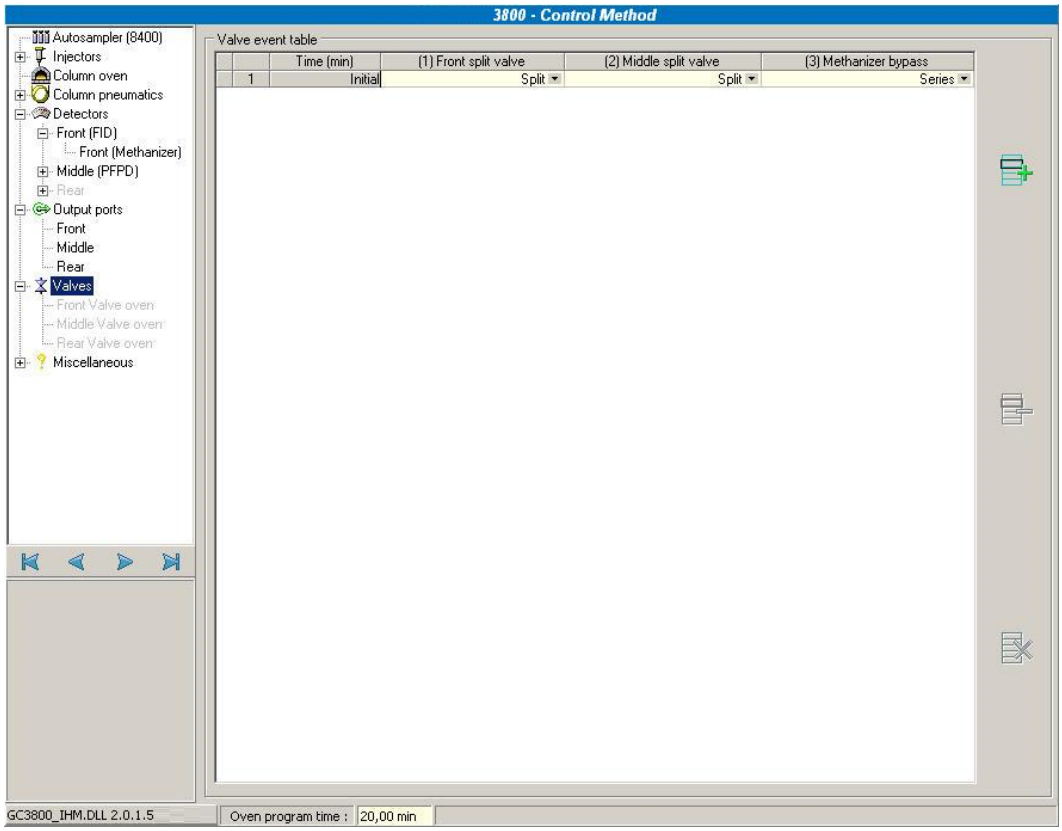
To add a line to the table.

To delete a line in the table.

To clear the entire table.

Valves Control

The 3800 GC can be configured with a wide variety of valves. The Valves window contains the valves table program (for sample delivery) and up to three valve oven programs:



Valve Event Table Parameter Group

Use the table to change valves settings during the analysis.

The first row of the table contains the initial setting for each valve. The remainder of the table contains the time-programmed settings: each valve will be switched to the value in each row at the indicated *Time*.

Use the following buttons to edit the table:

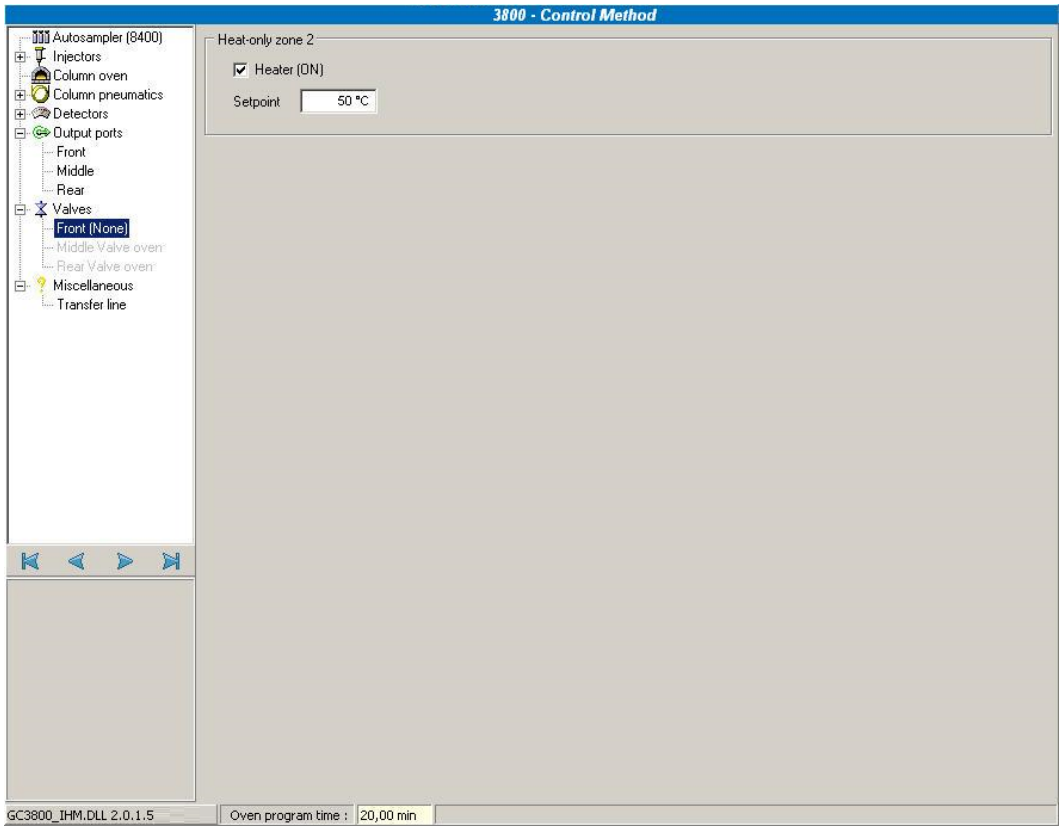
To add a line to the table.

To delete a line in the table.

To clear the entire table.

Valve type	Description
Split valve	Splitless or split The 3800 GC can have up to three split valves installed (Front, Middle, Rear)
Gas Sampling Valve	Fill or Inject
Liquid Sampling Valve	Fill or Inject
Sample	Off or On
Internal Standard	Off or On
Surrogate Standard	Off or On
Series Bypass	Series or Bypass
Backflush to Detector	Forward or Backflush
Backflush to Vent	Forward or Backflush
Column Selection	Column 1 or Column 2
Injection + Backflush to Detector	Fill and Backflush or Inject
Injection + Backflush to Vent	Fill and Backflush or Inject
Alternate Injection	Column 1 or Column 2
Simultaneous Injection	Fill or Inject
Methanizer Bypass	Series or Bypass
Sample Preconcentration Trap	SPT desorb or SPT trap
Event A, B, C, D	Off or On

If a valve oven is installed, click on it (Front, Middle or Rear) to display the corresponding window. The valve oven is an optional, isothermal heated zone.



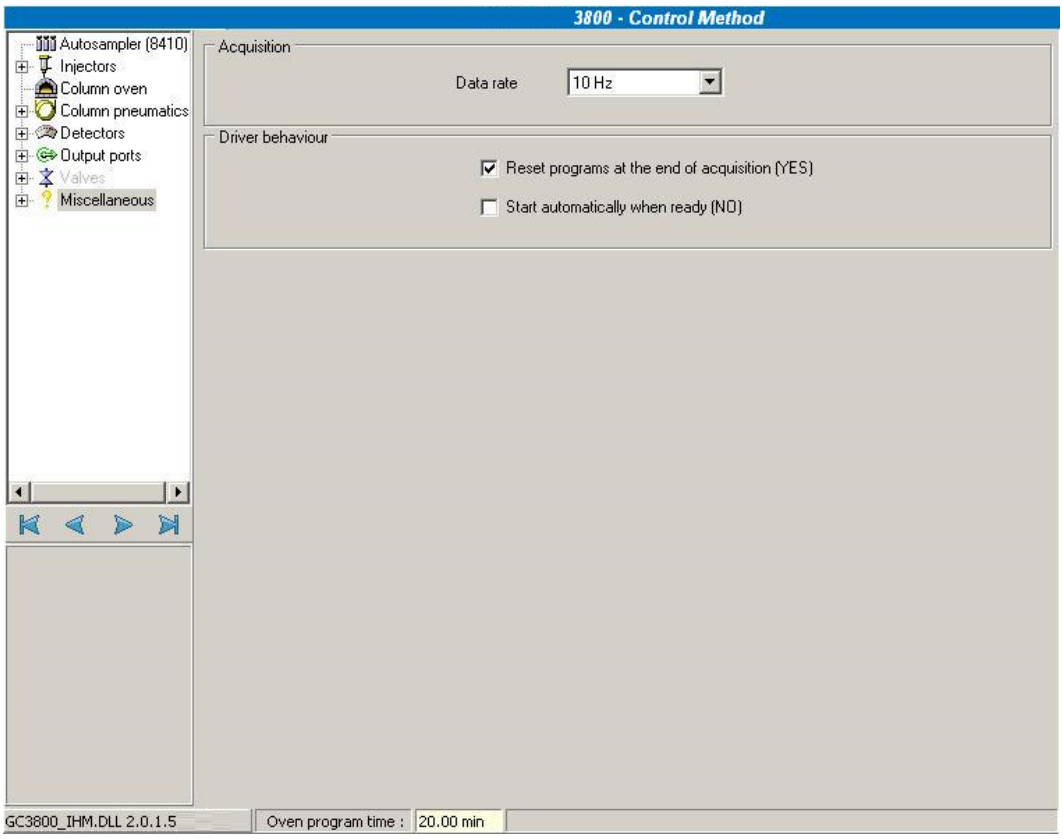
Heat-only Zone Parameter Group

Check or uncheck the *Heater* option to indicate whether or not you will use the installed valve.

Enter the isothermal temperature of the valve oven in the *Setpoint* field.

Miscellaneous

The Miscellaneous window contains parameters for data collection and transfer line:



Acquisition Parameter Group

Enter the detector data rate in the *Data rate* field. With decreased data rates, less disk space is required for storing the data. However, with increased rates, more data is collected, which may improve quantitation, particularly for narrow peaks.

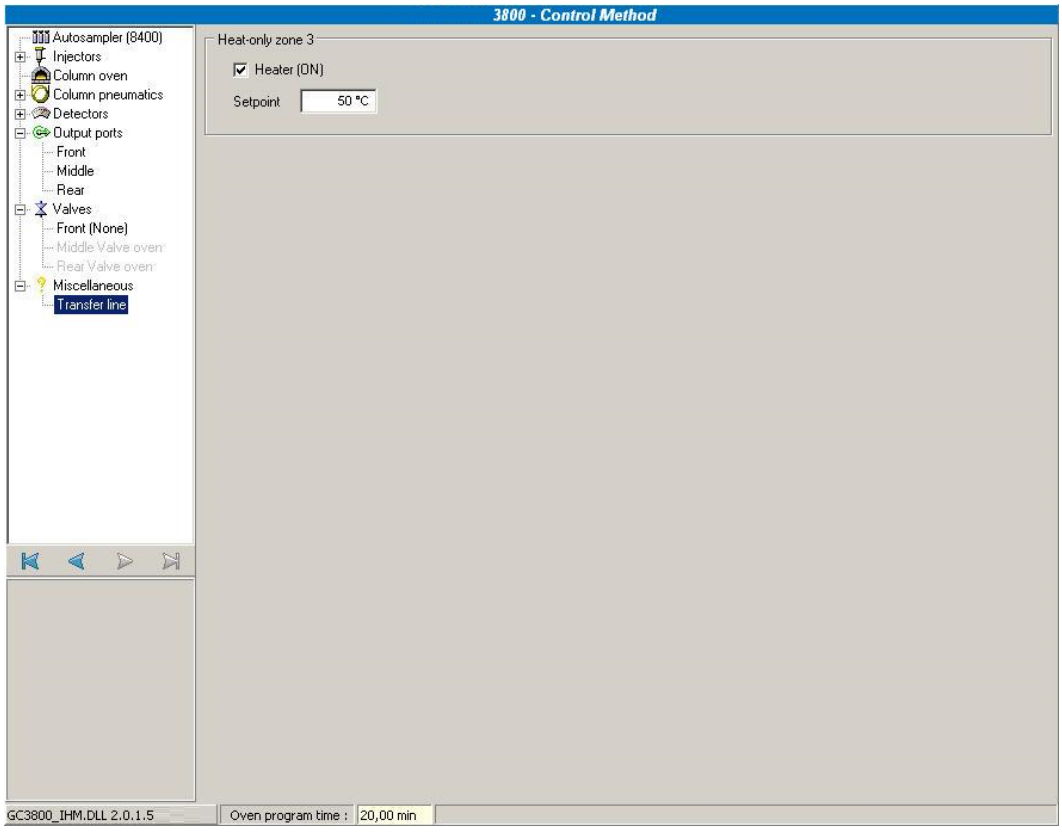
Driver Behavior Parameter Group

Check or uncheck the *Reset programs at the end of the acquisition* option to active it or not. If this option is checked and the acquisition is stopped from the acquisition window, the temperature programs will be reset before continuing with the next injection (if a sequence is running).

Check *Start automatically when ready* to start the GC without injecting. This could be useful in case of sampling valve use, for example.

Transfer Line

If a transfer line is installed, Check or uncheck the *Heater* option to indicate whether or not you will use it and enter the isothermal temperature of the transfer line in the *Setpoint* field:


3800 - Control Method
Autosampler (8400)
Injectors
Column oven
Column pneumatics
Detectors
Output ports
Front
Middle
Rear
Valves
Front (None)
Middle Valve oven
Rear Valve oven
Miscellaneous
Transfer line
Heat-only zone 3
Heater (ON)
Setpoint
50 °C
GC3800_IHM.DLL 2.0.1.5
Oven program time :
20,00 min

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

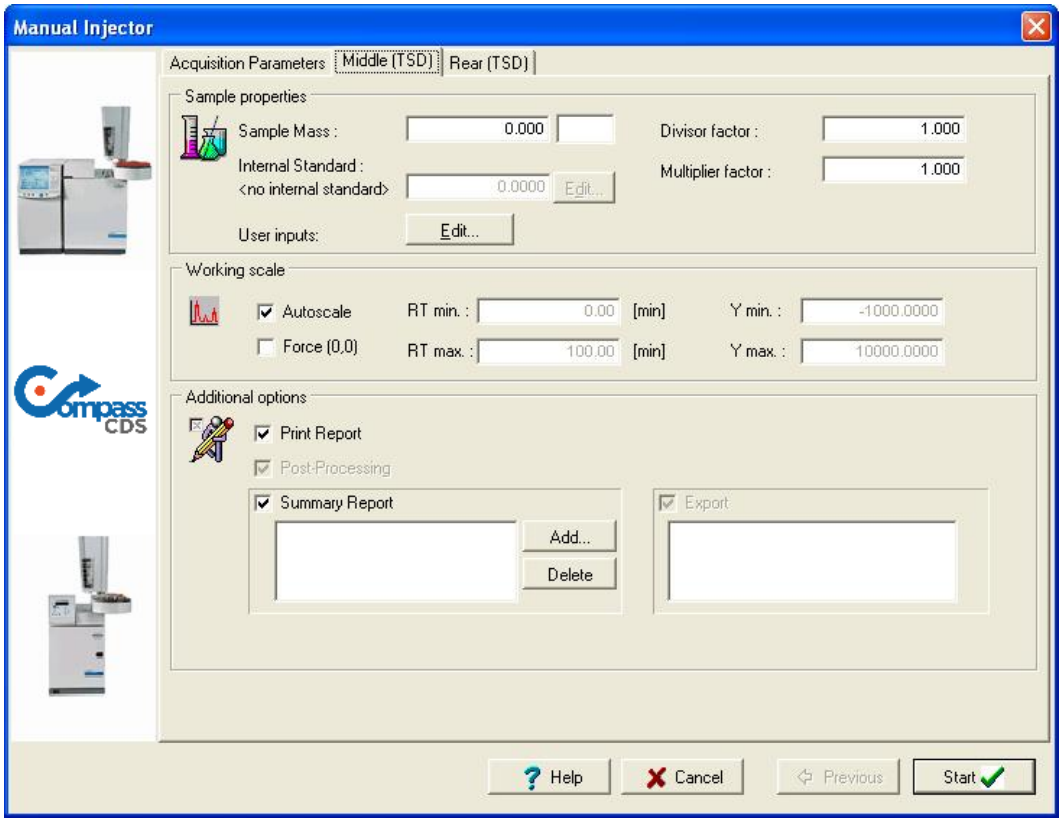
Quick Start (Single Acquisition)

1. Press the button.

   In the ***Quick Start*** window, select the system, the method and optionally the project if connected in "All project" mode.

2. Press the *OK* button.

   The following screen is displayed:



In the *Acquisition parameters* tab, required like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by compassCDS, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the *Channel X* tab.

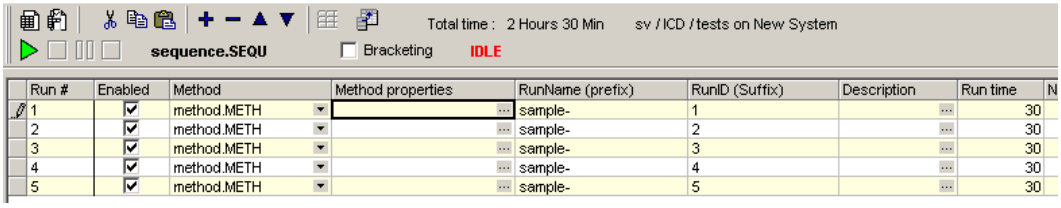
3. Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the

same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the *FILE / NEW SEQUENCE menu*, and complete the displayed creation wizard screen (refer to CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time
1	☑	method.METH		sample-	1		30
2	☑	method.METH		sample-	2		30
3	☑	method.METH		sample-	3		30
4	☑	method.METH		sample-	4		30
5	☑	method.METH		sample-	5		30

The *Method Name*, the *Run Name*, the *Run ID,* and the *Acquisition length* must be filled before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed. If Dual View is selected then the acquisition will be observed while the sequence is running.

Status of the 3800 GC

Click on the button corresponding to the 3800 GC driver and the 3800 GC status screen will appear. It contains nine sub-sections: *Autosampler*, *Injectors*, *Column oven*, *Columns*, *Detectors*, *Output ports*, *Valves*, *Miscellaneous*, and *Overview*. Click on the required sub-section to display the corresponding parameters that will be used during the chromatographic run.

A toolbar allows you to easily scroll through the status windows:

To select the first status window.

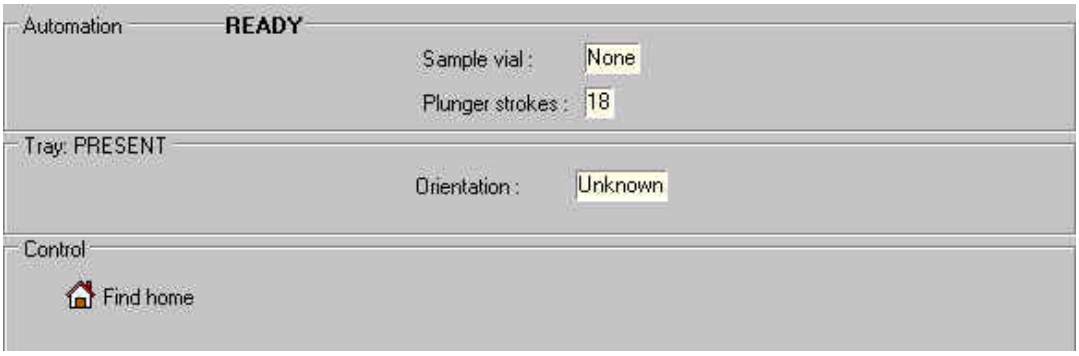
To move back to the previous status window.

To move forward to the next status window.

To select the final status window.

Autosampler Window

This option is only shown on 3800 GCs that have an 8400 AutoSampler or 8410 AutoInjector connected to them.



The Autosampler status screen indicates the autosampler state *(Ready, Running, Suspended, Resetting or Running Priority Sample).*

The display also includes the following parameters:

Sample vial*:* Corresponds to the current vial.

Plunger Strokes: Displays the number of times that the syringe plunger has been stroked up and down. This can be used to help monitor syringe wear and plan for syringe replacement.

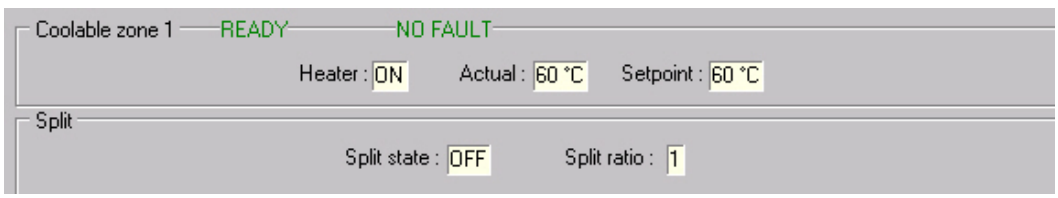
Present: Indicates whether the tray is present or not.

Orientation: Shows the range of vials accessible from the carrousel location (8410 AutoInjector Only)

Click on the

button to reinitialize the autosampler.

Injectors Window



The following status parameters are available for any injector type:

***Ready* or *Not ready*:** The injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the injector component has occurred.

Heater: Displays if the injector oven component is turned OFF or ON at the 3800 GC.

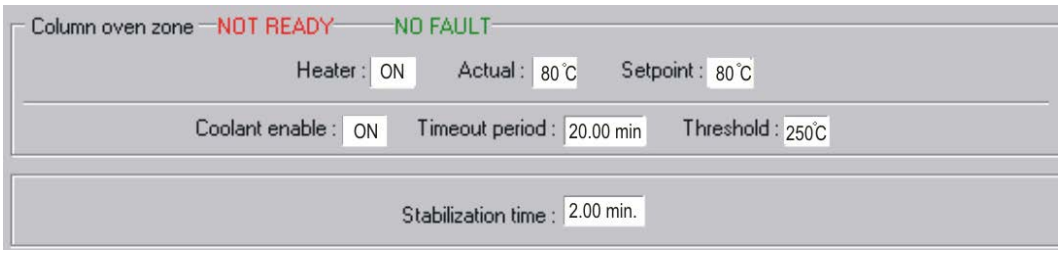
***Actual*:** Displays the actual temperature of the injector oven at the 3800 GC.

Setpoint: Displays the injector oven programmed temperature setting in the active method.

Other parameters can be displayed according to the injector type:

Injector	Parameter	Description
1079	*Coolant Enable*	Displays if the 1079 injector oven coolant is enabled in the active method.
	Timeout Period	Displays the programmed coolant time-out value in the active method for the 1079 injector oven.
	Threshold	Displays the programmed injector oven temperature at which the 1079 injector oven coolant is enabled.
	Split State	Displays the current split state of the 1079 injector method.
	Split Ratio	Displays the current split ratio of the 1079 injector method. The split ratio is defined as the (Column Flow + the Split Flow) / the Column Flow.
1177	*Split State*	Displays the current split state of the 1177 injector method.
	Split Ratio	Displays the current split ratio of the 1177 injector method. The split ratio is defined as the (Column Flow + Split Flow) / the Column Flow.
SPT	*Coolant Enable*	Displays if the SPT injector oven coolant is enabled in the active method.
	Threshold	Displays the programmed injector oven temperature at which the SPT injector oven coolant is enabled.
	Timeout Period	Displays the programmed coolant time-out value in the active method for the SPT injector oven.

Column Oven Window



The status display includes the following parameters:

***Ready* or *Not Ready*:** The column oven is Ready if the setpoints have been achieved and stabilized. The column oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance.

NOTE: Some reasons the GC may go Not Ready during a run are: the temperature program is too aggressive, the oven door is opened, the coolant runs out, the power line voltage drops, etc.

Fault: Displays if a fault in the column oven component has occurred.

Heater: Displays if the column oven component is turned OFF or ON at the 3800 GC.

Actual**:** Displays the actual temperature of the column oven at the 3800 GC.

Setpoint: Displays the column oven programmed temperature setting in the active method.

Coolant enable: Displays if the column oven coolant is enabled in the active method.

Threshold**:** Displays the programmed column oven temperature at which the column oven coolant is enabled.

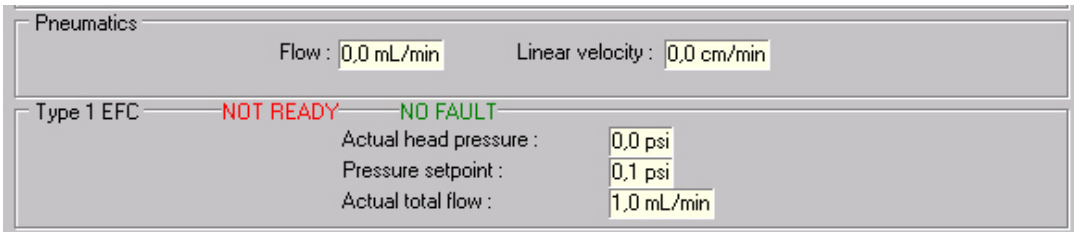
Timeout period**:** Displays the programmed coolant time-out value in the active method for the column oven.

Stabilization time: Shows the 3800 GC column oven stabilization time in minutes. The stabilization time counts down from the programmed method value and then displays 0.00 minutes when the stabilization period is over.

Column Window

The columns status screen depends on the installed EFC modules.

Type 1 EFC Status Screen



The status display includes the following parameters:

Ready* or *Not Ready**:** The Type 1 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 1 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

Fault* or *No Fault**:** Displays if a fault in the Type 1 EFC component has occurred.

Flow**:** Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

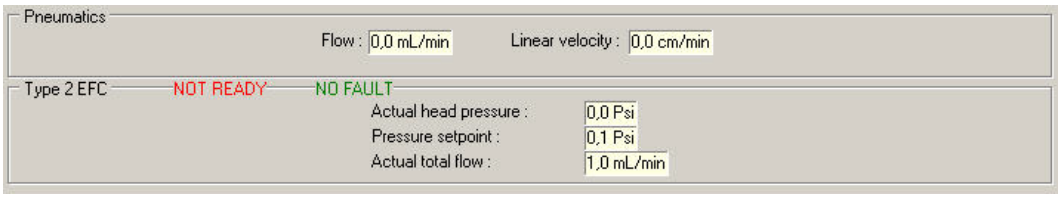
Linear Velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual Head Pressure: Displays the actual column head pressure at the 3800 GC.

Pressure Setpoint: Displays the programmed column head pressure setting in the active method.

Actual Total Flow: Displays, in mL/min, the total flow rate through the system.

Type 2 EFC Status Screen



The status display includes the following parameters:

***Ready* or *Not Ready*:** The Type 2 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 2 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the Type 2 EFC component has occurred.

***Flow*:** Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

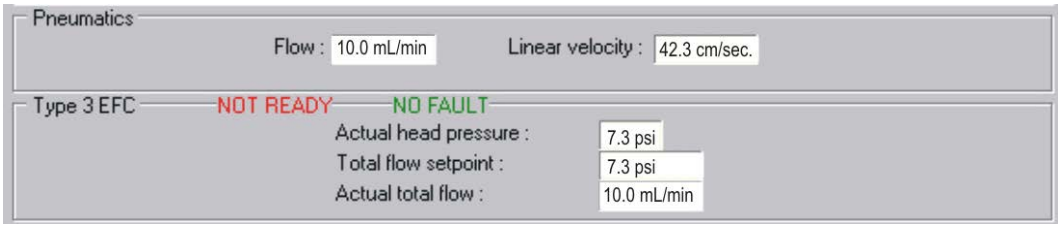
***Linear Velocity*:** Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

***Actual Head Pressure*:** Displays the actual column head pressure at the 3800 GC.

***Pressure Setpoint*:** Displays the programmed column head pressure setting in the active method.

***Actual Total Flow*:** Displays, in mL/min, the total flow rate through the system.

Type 3 EFC Status Screen



The status display includes the following parameters:

***Ready* or *Not Ready*:** The Type 3 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 3 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the Type 3 EFC component has occurred.

***Flow*:** Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

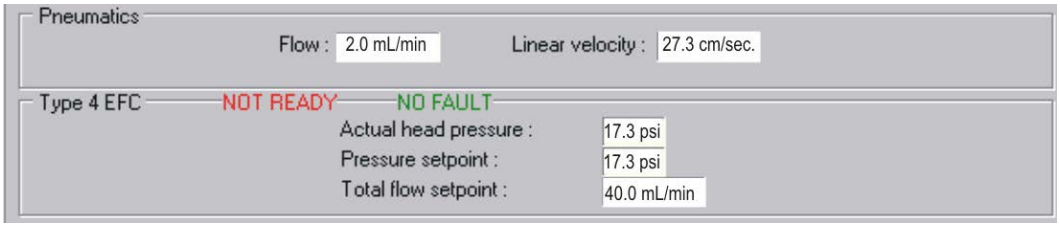
Linear Velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual Head Pressure: Displays the measured column head pressure at the 3800 GC.

Total Flow Setpoint: Displays the programmed total flow rate setting in the active method.

Actual Total Flow: Displays, in mL/min, the actual total flow rate.

Type 4 EFC Status Screen



The status display includes the following parameters:

***Ready* or *Not Ready*:** The Type 4 Injector EFC component is Ready if the setpoints have been achieved and stabilized. The Type 4 Injector EFC component is Not Ready if readiness to start a run has not been achieved or if, during a run, the EFC becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the Type 4 EFC component has occurred.

Flow: Displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Linear Velocity: Displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Actual Head Pressure: Displays the actual column head pressure at the 3800 GC.

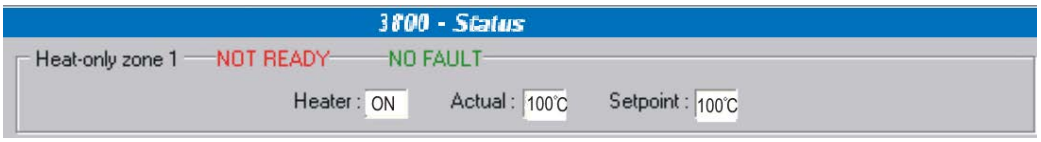
Pressure Setpoint: Displays the programmed column head pressure setting in the active method.

Total Flow Setpoint: Displays, in mL/min, the programmed total flow rate in the active method.

Detectors Window

The detector status screen depends on the installed detector.

The following parameters are available for all the detectors:



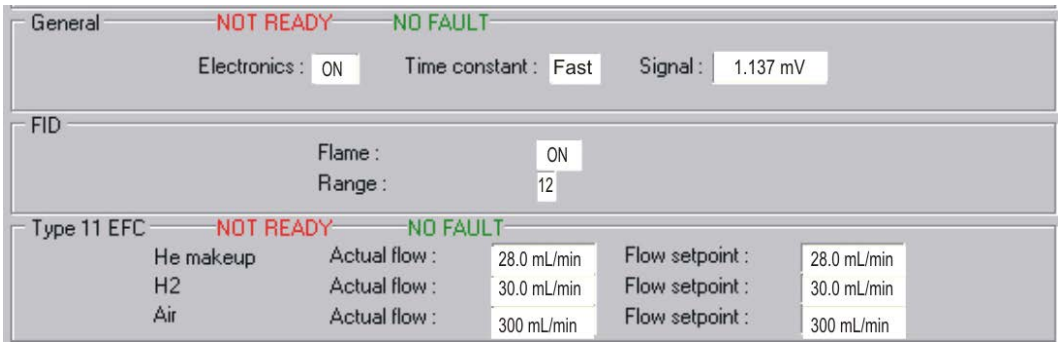
Heater: Displays if the injector oven component is turned OFF or ON at the 3800 GC.

***Actual*:** Displays the actual temperature of the injector oven at the 3800 GC.

Setpoint: Displays the injector oven programmed temperature setting in the active method.

Some other parameters are dependent of the type of detector:

FID Status Screen



The status display includes the following parameters:
***Ready* or *Not Ready*:** The FID detector is Ready if the setpoints have been achieved and stabilized. The FID detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the FID detector becomes not ready or goes out of tolerance.

Fault* or *No Fault: Displays if a fault in the FID detector component has occurred.

***Electronics*:** Displays the FID Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual FID detector signal at the 3800 GC.

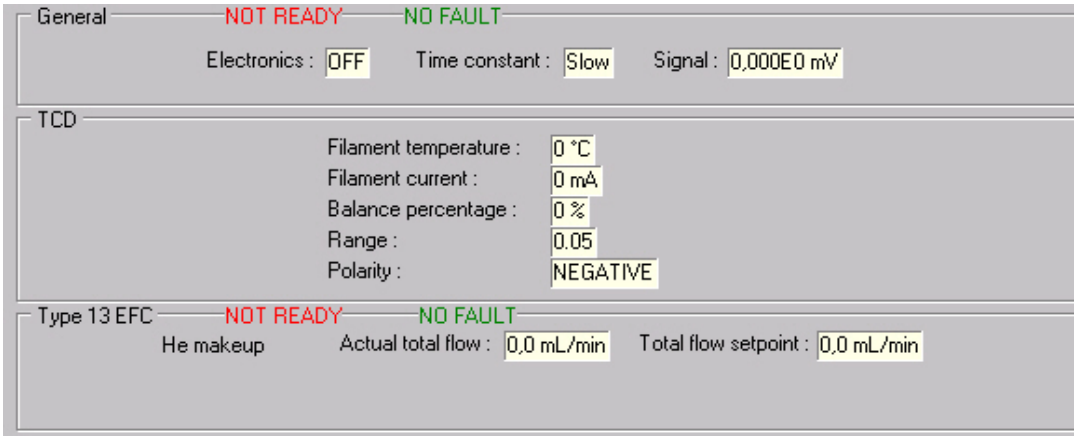
Flame: On or Off.

***Range*:** 9, 10, 11, or 12. Displays the FID Range initial condition setting or the time-programmed setting in the active method.

If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and displays the following parameters:

EFC Type	Parameters	Description
Type 11 EFC	*Ready*	Or Not Ready.
	Fault	Or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

TCD Status screen



The status display includes the following parameters:
***Ready* or *Not Ready*:** The TCD detector is Ready if the setpoints have been achieved and stabilized. The TCD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the TCD detector becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the TCD detector component has occurred.

***Electronics*:** Displays the TCD Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual TCD detector signal at the 3800 GC.

Filament Temperature: Displays the TCD Filament Temperature setting in the active method.

Filament Current: Displays, in mA, the actual TCD current.

Balance Percentage: Displays, in %, the TCD bridge balance.

NOTE: On the 3800 GC, the bridge is balanced automatically when autozero is executed, and should normally set around 0 - 5%. A large offset in bridge balance (+ or -) could indicate a potential problem.

Range: 0.05, 0.5, or 5.0. Displays the current TCD Range.

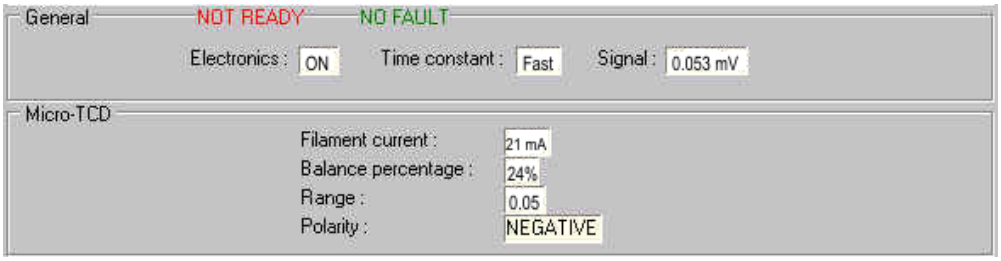
Polarity: Displays the current TCD Polarity.

If the detector Electronic Flow Control module is installed, the Type XY EFC section will appear. Three EFC modules can be used with the TCD detector.

The table below shows the corresponding EFC status items:

EFC Type	Parameters	Description
Type 13 EFC	*Ready*	Or Not Ready.
	Fault	Or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
Type 14 EFC	*Ready*	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Helium, Nitrogen, or Argon make up.
	Reference	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Helium, Nitrogen, or Argon reference.
Type 16 EFC	*Ready*	or Not Ready.
	Fault	or No Fault. Displays if a fault in the EFC module has occurred.
	Makeup	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Hydrogen make up.
	Reference	Displays, in mL/min, the setpoint and actual channel 2 flow rate if channel 2 is configured as Hydrogen reference.

Micro-TCD Status Screen



The status display includes the following parameters:
***Ready* or *Not Ready*:** The Micro-TCD detector is Ready if the setpoints have been achieved and stabilized. The Micro-TCD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the Micro-TCD detector becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the Micro-TCD detector component has occurred.

***Electronics*:** Displays the microTCD Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual Micro-TCD detector signal at the 3800 GC.

Filament Current: Displays, in mA, the actual Micro-TCD current.

Balance percentage: Displays, in %, the Micro-TCD bridge balance.

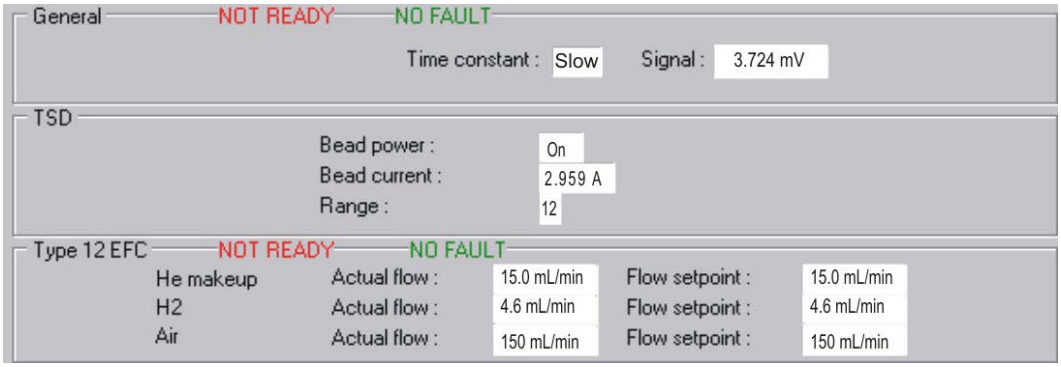
NOTE: On the 3800 GC, the bridge is balanced automatically when autozero is executed and should normally set around 0%.A large offset in bridge balance(+ or -) could indicate a potential problem.

Range: 0.05, 0.5, or 5.0. Displays the current Micro-TCD Range.

Polarity: Displays the current Micro-TCD Polarity.

NOTE: The Micro-TCD detector temperature is set to 110 °C and is not user adjustable.

TSD Status Screen



The status display includes the following parameters:

***Ready* or *Not Ready*:** The TSD detector is Ready if the setpoints have been achieved and stabilized. The TSD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the TSD detector becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the TSD detector component has occurred.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: Displays, in mV, the actual TSD detector signal at the 3800 GC.

Bead Power: Displays the current TSD Bead Power.

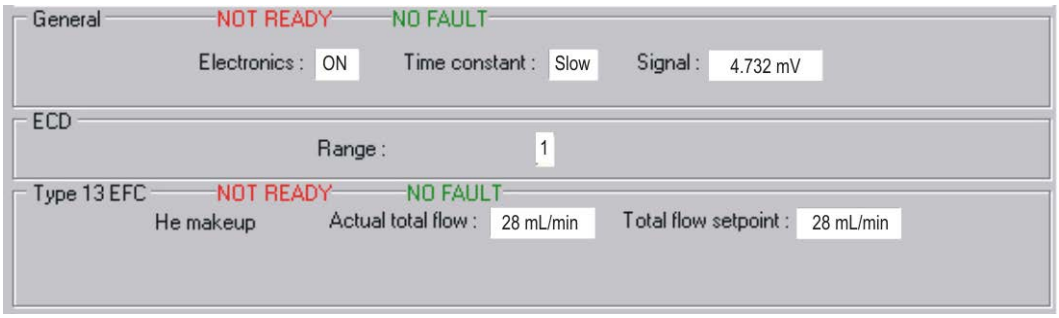
Bead Current: Displays the TSD Bead Current setting in the active method.

Range: 9, 10, 11, or 12. Displays the current TSD Range.

If the detector Electronic Flow Control module is installed, the Type 12 EFC section will appear and displays the following parameters:

EFC Type	Parameters	Description
Type 12 EFC	*Ready*	Or Not Ready.
	Fault	Or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

ECD Status Screen



The status display includes the following parameters:
***Ready* or *Not Ready*:** The ECD detector is Ready if the setpoints have been achieved and stabilized. The ECD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the ECD detector becomes not ready or goes out of tolerance.

***Fault* or *No Fault*:** Displays if a fault in the ECD detector component has occurred.

***Electronics*:** Displays the ECD Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

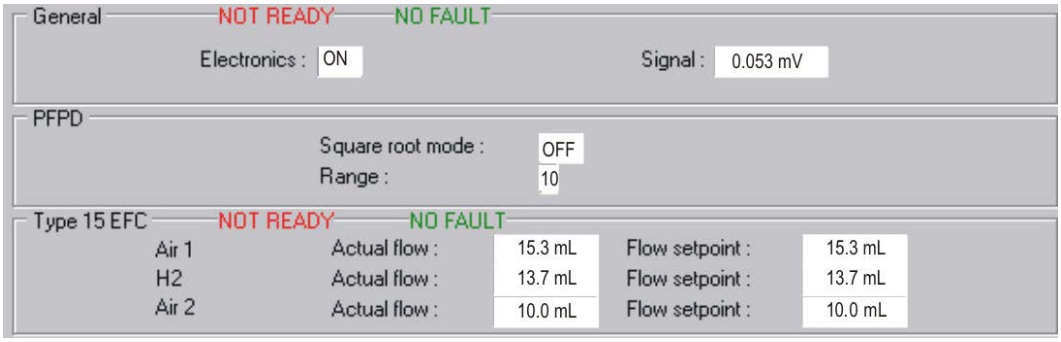
Signal: Displays, in mV, the actual ECD detector signal at the 3800 GC.

Range: 1 or 10. Displays the current ECD Range.

If the detector Electronic Flow Control module is installed, the Type 13 EFC section will appear and displays the following parameters:

EFC Type	Parameters	Description
Type 13 EFC	*Ready*	Or Not Ready.
	Fault	Or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate

PFPD Status Screen



The status display includes the following parameters:
***Ready* or *Not Ready*:** The PFPD detector is Ready if the setpoints have been achieved and stabilized. The PFPD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the PFPD detector becomes not ready or goes out of tolerance.

Fault* or *No Fault: Displays if a fault in the PFPD detector component has occurred.

***Electronics*:** Displays the PFPD Electronics setting in the active method.

Signal: Displays, in mV, the actual PFPD detector signal at the 3800 GC.

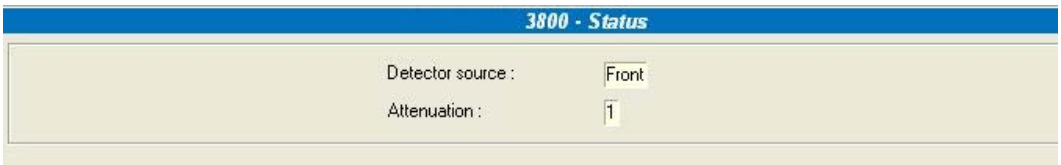
Square Root Mode: Displays the PFPD Square Root Mode setting in the active method.

Range: 8, 9 or 10. Displays the current PFPD Range.

If the detector Electronic Flow Control module is installed, the Type 15 EFC section will appear and displays the following parameters:

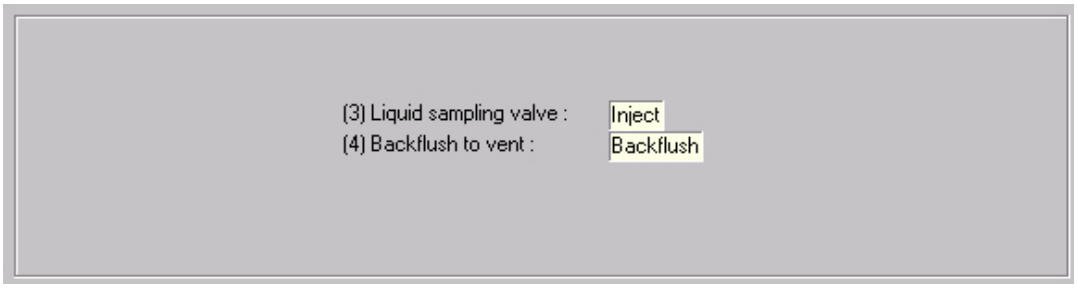
EFC Type	Parameters	Description
Type 15 EFC	*Ready*	Or Not Ready.
	Fault	Or No Fault. Displays if a fault in the EFC module has occurred
	Makeup	Displays, in mL/min, the setpoint and actual channel 1 flow rate
	H_2	Displays in mL/min, the setpoint and actual channel 2 flow rate
	Air	Displays, in mL/min, the setpoint and actual channel 3 flow rate.

Output Ports Window



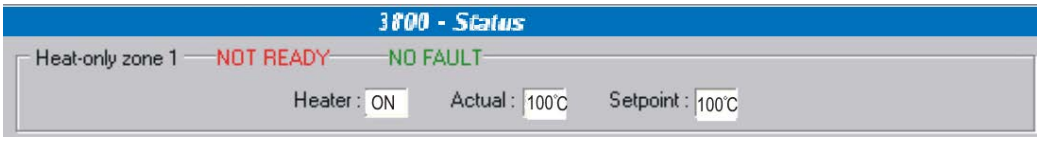
The status screen displays the actual *Detector source* and A*ttenuation* for the corresponding port.

Valves Window



If the valves are configured, the status displays the assigned valve name and current state at the 3800 GC.

If a valve oven is installed, the status displays the following parameters:



Heater: Displays if the valve oven is turned OFF or ON at the 3800 GC.

***Actual*:** Displays the actual temperature of the valve oven at the 3800 GC.

Setpoint: Displays the valve oven temperature setting in the active method.

Miscellaneous Window

The miscellaneous screen contains general information about the current run and the overall state of the instrument.

The state of the instrument (Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready) is displayed.

A Fault / No Fault indicator is also shown. When a hazardous or disabling fault occurs, any run in progress will halt and the affected component will shut down. If the fault is recoverable, then the run is not terminated.

The active method number in the GC is displayed with the current *Data rate*.

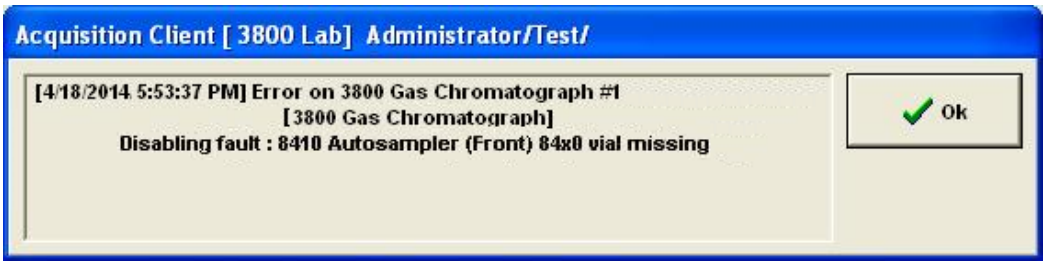
The run time bar displays the elapsed time in minutes since the beginning of the run and the end time.

If the coolant option is timed out, Yes will appear in the corresponding *Coolant timed out* field to indicate a fault has occurred.

Press the Reset programs button, in the *Control* field, to reset the GC. If it is *RUNNING*, the GC aborts the current run , goes to the READY state and continues with the next injection in the sequence. This button is equivalent to pressing the Stop on the front panel of the GC.

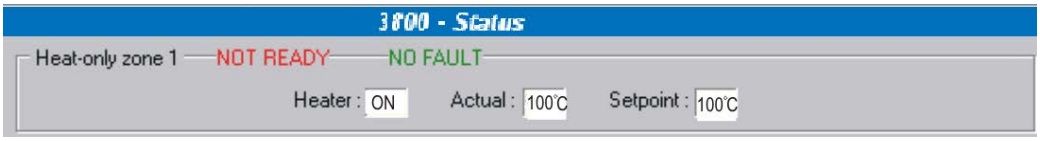
When a vial is missing during a sequence, a warning message appears and you have 10 minutes to replace the sample in the correct position before the system skips the missing vial and passes to the next line of the sequence, or stops the run. When you have replaced the missing sample, you must press the Re-inject button to restart the run.

If you want to skip the missing vial and start the next run, you must press the Skip vial button.


Acquisition Client [3800 Lab] Administrator/Test/
[4/18/2014 5:53:37 PM] Error on 3800 Gas Chromatograph #1
[3800 Gas Chromatograph]
Disabling fault : 8410 Autosampler (Front) 84x0 vial missing
Ok

Warning message when a vial is missing.

If a transfer line is installed, the status displays the following parameters:



Heater: Displays if the transfer line is turned OFF or ON at the 3800 GC.

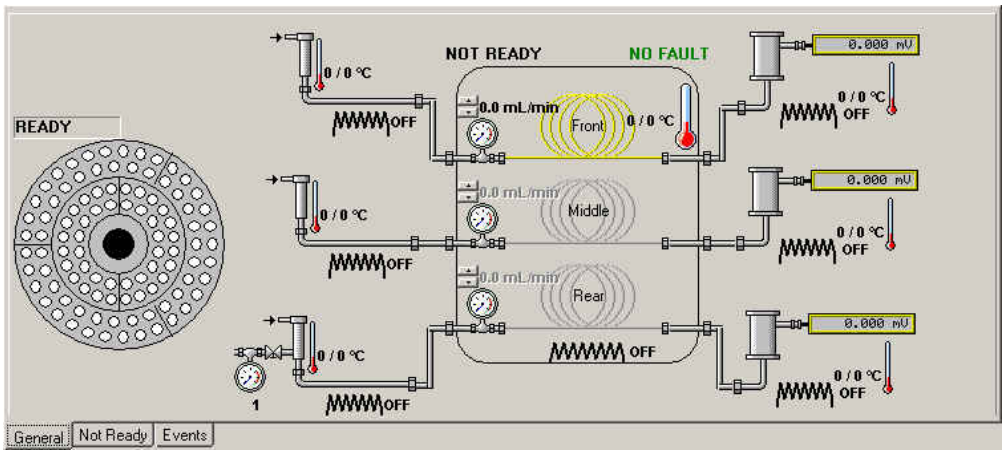
***Actual*:** Displays the actual temperature of the transfer line at the 3800 GC.

Setpoint: Displays the transfer line temperature setting in the active method.

Overview Window

Click on the Over View button: the ***Status Overview*** window is displayed and contains three tabs:

- *General:* displays the synopsis of the GC, where some current values can be read (temperatures, pressures, signal, etc.).



When the mouse points to a colored vial (yellow for current vial, green for already used vial, and red for missing vial), the current vial number and the number of injections are displayed.

The flow and temperature (current and setpoint) for each module and the signal values are displayed. You can choose to display the flow, the pressure or the velocity of the gas in the column by clicking on the button.

- *Not Ready:* contains the not ready information sent by the GC.
- *Events:* contains the events that have occurred on the instrument, listed below:

3800 GC Faults:

Air Leak Fault	The 3800 GC just detected that the specified TCD has a disabling air leak.
Board Failure	The 3800 GC just detected that the specified PFPD has a failed electronics board.
Coolant Timed Out	The 3800 GC just detected that the specified component temperature zone coolant has timed out.
Data loss due to workstation disconnect	The 3800 GC just detected that its raw data buffer has overflowed because it was unable to transmit its contents to the CompassCDS Chromatography Data System workstation quickly enough.
Flame-out	The 3800 GC just detected that the specified FID has a flame-out. The flame detection is based on a background signal intensity of approximately 330 micro volts. It is possible for very clean GC systems to have baselines less than 330 micro volts causing spurious flameout messages. If you suspect that the flameout message is spurious, use a shiny, cool metal object (such as a box end wrench) and hold it just above the FID tower, being careful not to get too close to the hot surfaces. If you observe condensation, then the flame is still lit; you may wish to change your fuel gas mixture or some other operating characteristic that would allow a slightly higher background signal. Once a flame out is detected, the system will attempt to ignite the flame 3 times before reporting the flame out condition. The fault is cleared by turning the Detector electronics off and on, or by igniting the flame. Alternatively, you may disable the flame-out detection in the setup, miscellaneous section of the 3800.
Gas saver timeout expired	The GC has been idle for a period of time equal to or greater than the set Gas Saver timeout period. Activate a method to clear the fault
Large Air Leak	The 3800 GC just detected that the specified TCD has a large air leak.
Lower than minimum specified temp	The 3800 GC just detected that the specified component temperature zone has gone below its minimum temperature.
Max setup temperature limit exceeded	The 3800 GC just detected that the specified component temperature zone has exceeded its maximum setup temperature limit.
Maximum temp has been exceeded	The 3800 GC just detected that the specified exceeded component temperature zone has exceeded its maximum temperature.
No response from temp probe	The 3800 GC just detected that the specified component temperature zone probe is not responding.
Temp probe is open	The 3800 GC just detected that the specified component temperature zone probe has an open circuit.
Temp probe is shorted	The 3800 GC just detected that the specified component temperature zone probe has a short circuit.
Temp probe response is too fast	The 3800 GC just detected that the specified component temperature zone probe is responding too fast.
Temp probe response is too slow	The 3800 GC just detected that the specified component temperature zone probe is responding too slowly.
Thermal runaway	The 3800 GC just detected that the specified component temperature zone has begun thermal runaway.
Workstation connected	The 3800 GC just detected that the CompassCDS Chromatography Data System workstation has connected its Ethernet communications.
Workstation disconnected	The 3800 GC just detected that the CompassCDS workstation has disconnected its Ethernet communications.

Autosampler Faults:

84x0 communication	The AutoSampler/AutoInjector has experienced an error during communications that was unrecoverable. Power off both your GC and the autosampler. Turn on power to the GC followed by turning on the power to the autosampler.
84x0 faulted	The autosampler has failed to properly come up. Turn off the power and then turn it back on.
84x0 carrousel error	The autosampler carrousel base has encountered one or more internal faults and has failed to properly come up. Turn off the power and then turn it back on.
84x0 maximum plunger exceeded	This message is displayed if you have built a speed method with one syringe that supports a fast injection speed and have subsequently changed and configured a different syringe. Correct the syringe speed in your method for the new syringe
84x0 plunger error	The syringe plunger has either jammed or become inoperable. Check that the syringe is properly mounted and that you have free movement of the plunger. Replace the syringe if required.
84x0 run ended before the injection sequence.	The autosampler failed to complete second injection Restart Automation to clear the fault.
84x0 run not started after injection	Restart Automation to clear this fault. If it recurs, check that the inject switch installed on the injector nut is functioning properly.
84x0 syringe sled error	The syringe sled is either jammed or miscalibrated. Recalibrate your vial and injector positions making sure that the syringe sled has a small clearance (consult your manual) above vials and does not compress the injector switch on the injector.
84x0syringe volume exceeded	The total volume of the sample, air gaps (if any), solvent plugs (if any), and internal standards (if any) exceeds the capacity of the configured syringe. Note that this error is only sensed at the time of injection. Check your method and correct any volumes that are excessive.
84x0 tower error	The autosampler tower has one or more internal faults and has failed to properly come up. Turn off the power and turn it back on.
84x0 tray is missing	The CP-8410 sample tray has been removed from the base. Replace the tray; the CP-8410 should automatically sense that the tray has been replaced.
84x0 vial missing	The autosampler has failed to detect a vial within an expected range of vials. This message is an advisory message. If you have a vial in the position and it has been missed, check that a septum is installed. Lack of a septum and dark colors may cause the tower sensor to fail to identify the vial.
84x0vial sensor bad	The autosampler vial sensor has failed to conform to its expected operation. Turn off the GC and turn it on again.

Varian 3900 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501493
Revision D

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the GC Communications 3
    Ethernet Communications 3
  Configuring the Driver 5
    Configuring the 3900 GC 5
    Configuring the Synopsis 21
Building a Method 24
  Creating a New Method 24
  Control Method Section for the 3900 GC 25
    Autosampler Control 26
    Injector Control 31
    Column Oven Control 33
    Column Pneumatics Control 34
    Detector Control 37
    External Events Control 41
    Miscellaneous Control 42
Starting and Viewing an Acquisition 43
  Quick Start and Sequence 43
    Quick Start (Single Acquisition) 43
    Sequence 44
  Running Acquisition Status 45
    Viewing a Running Acquisition 45
    Status of the 3900 GC 45
3900 GC Faults 54
Autosampler Faults 55

Introduction

This document describes the configuration of the Varian 3900 GC driver. It also explains how to build a control method for this driver, how to start and view a running acquisition, and what actions are available during an analysis.

The 3900 GC has a single 1177 split/splitless or a 1041 injector equipped with Injector Electronic Flow Control, an FID or a TCD detector with Electronic Flow Control, and optionally, a keypad and Ethernet communications.

CompassCDS Configuration Manager allows you to configure the 3900 GC without a keypad for the appropriate column dimensions and temperature limits, and to perform EFC and autosampler calibrations. All these functions can be accomplished locally when the 3900 GC is equipped with a keypad.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to CompassCDS installation Guide.

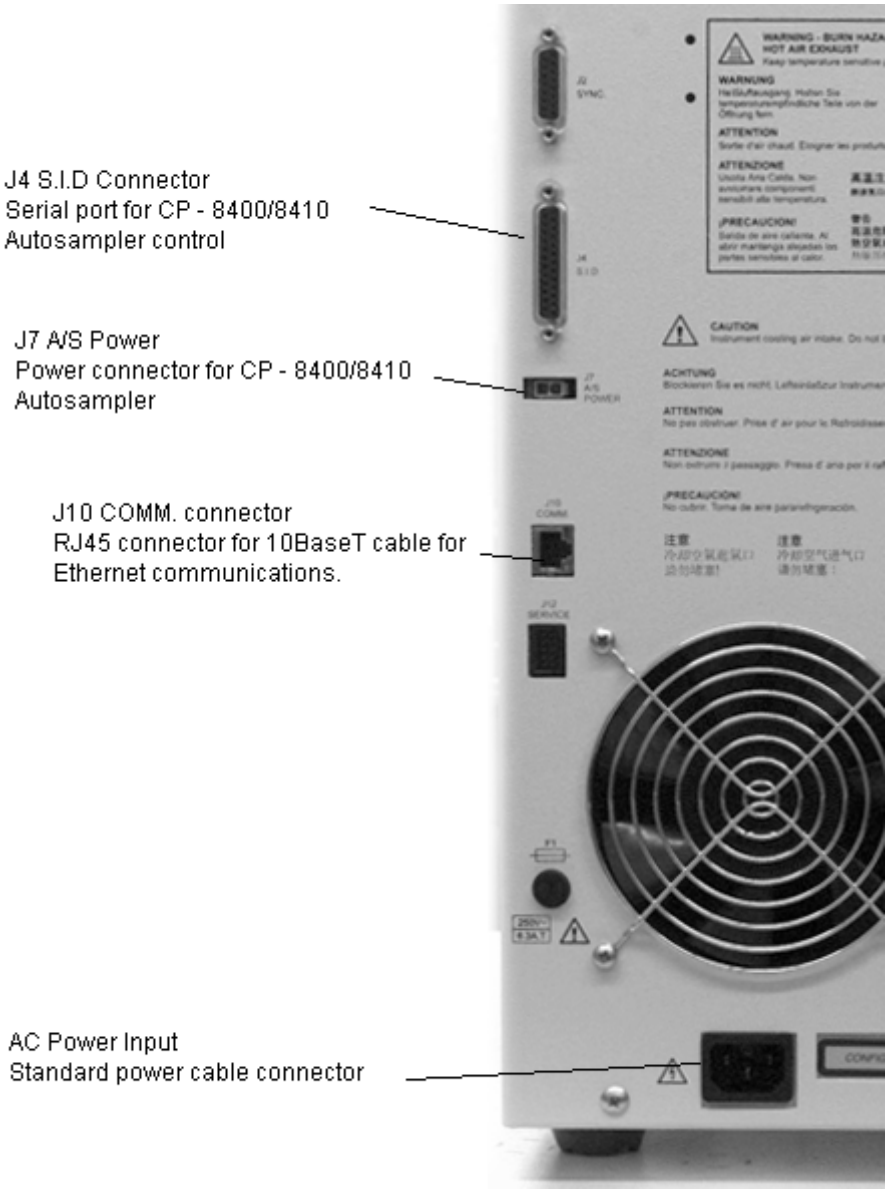
Configuring the GC Communications

Ethernet Communications

The 3900 Gas Chromatograph uses Ethernet® as the method of communication for instrument control and for sending digital data to the external data system.

The Ethernet connection is made at the back at the 3900 GC (J10 COMM. connector). There are two types of Ethernet cables:

- An Ethernet crossover cable is used when the 3900 GC is connected directly to the CompassCDS PC and the PC is not connected to a company network.
- A standard Ethernet patch cable is used when the 3900 GC is connected to a company Ethernet network. In this case, you will need to use an Ethernet 10BaseT hub or switch.



The 3900 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server is used to send IP addresses to TCP/IP devices.

The BOOTP Server lists Ethernet (MAC) addresses along with the IP addresses that are to be assigned to the corresponding devices.

To configure the BOOTP server, refer to the CompassCDS installation Guide.

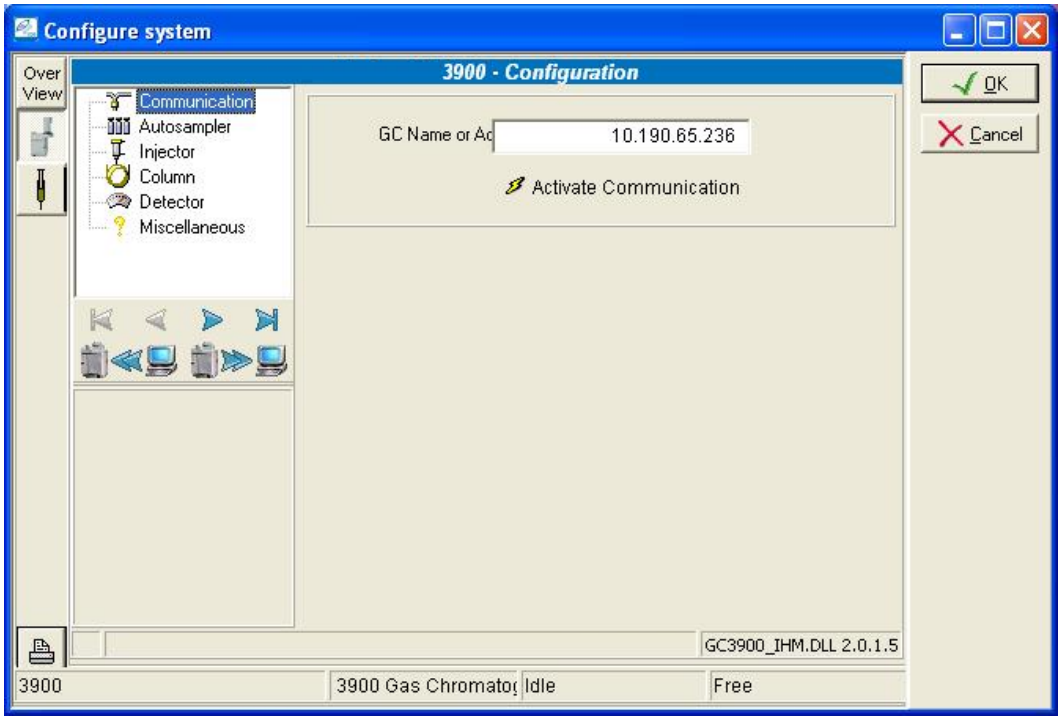
NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the 3900 GC

Click on the button corresponding to the 3900 GC driver and the GC configuration screens appear:



The toolbar allows you to easily scroll through the configuration windows:

to select the first configuration window.

to select the previous configuration window.

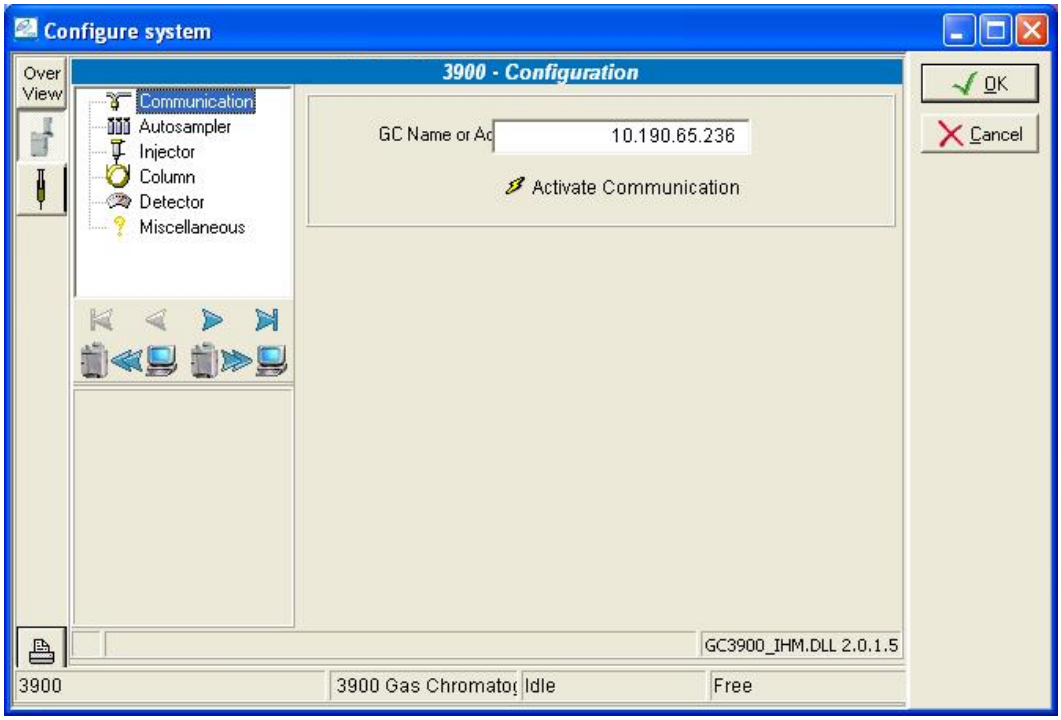
to select the next configuration window.

to select the final configuration window.

to send the configuration to the instrument.

to receive the configuration from the instrument.

Communication Window

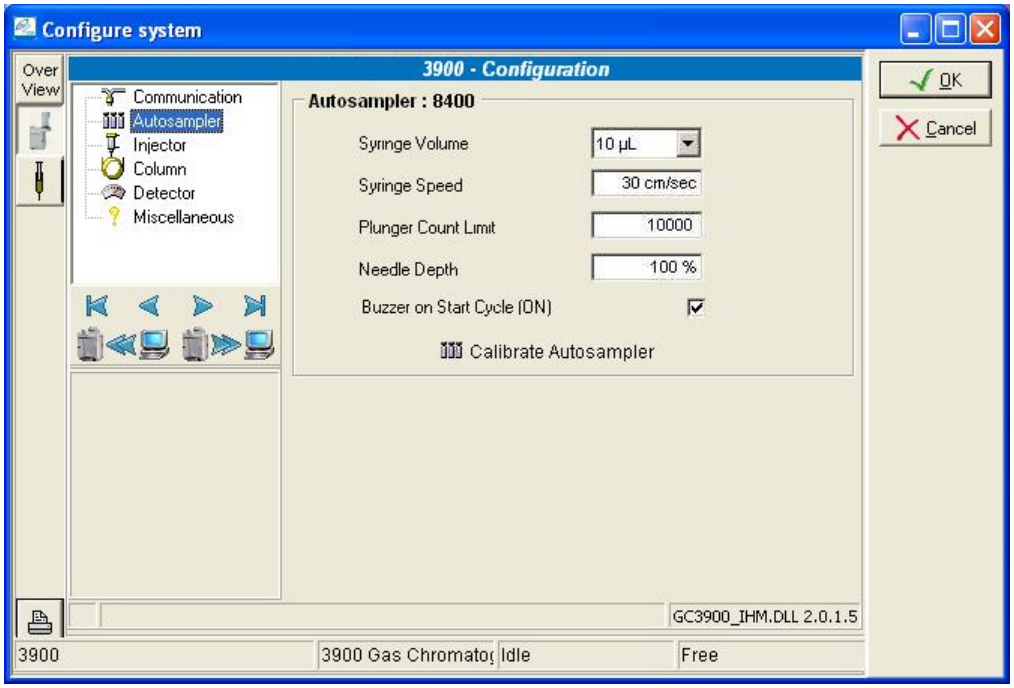


Enter the IP address of the 3900 (declared in the BOOTP Server) in the GC Name or Address field or click on the button to find the instrument previously declared with the BOOTP Server program and select it.

Press the

button to automatically get the configuration from the instrument.

Autosampler Window



Select volume (5, 10 or 100 µL) of the syringe you will install. The 3900 will use this value to set the correct entry selections and any needed internal setting to correctly use the indicated syringe size.

Enter the Syringe Speed (1 to 30 cm/sec, default = 30) in the corresponding field. The injector injection speed parameters define the rate at which the needle will penetrate the injector septum and descend to the set injector needle depth.

Enter the Plunger Count Limit (0 to 100 000, default = 10000): this parameter defines the number of strokes the plunger is expected to survive without significant degradation. Once the entered value is exceeded, a message will be displayed on the GC autosampler status, indicating the plunger counter has exceeded the set value.

Enter the Needle Depth (0 to 100%, default = 100) in the corresponding field. This parameter defines how far the needle will penetrate into the designated injector. 100 % causes the needle to be completely inserted to its 2-inch length.

Check the Buzzer on Start Cycle option to enable the buzzer: a sound will be generated to warn of impending tower movements when this parameter is set to On (default value).

Press the

button to calibrate the autosampler.

NOTE: The autosampler type is automatically detected by the CompassCDS driver.

Autosampler Calibration

If your 3900 GC is not equipped with a keypad, the calibration will be performed using the CompassCDS Configuration Manager. The goal of the calibration procedure is to align the autosampler needle with the first vial and with the injector.

NOTE: One basic rule associated with the calibration concerns rotation of the tower and carousel; to assure consistent operation, always approach the final calibration position with clockwise movements. To help facilitate this rule, the carousel will back up 10 steps when a counterclockwise action is selected but will move one step when a clockwise action is selected.

Vial Calibration:

1. To start the vial 0 (or vial 1 if 8410) calibration, make sure a vial with the same form factor and cap as the ones you will be using for your analyses is placed in the 0 position of the carousel (or the vial 1 position for the 8410).

2. Press the Start Calibration (F1) button (or the F1 key) in the *Calibrate Vial 0* (or *1*) *Position* field.

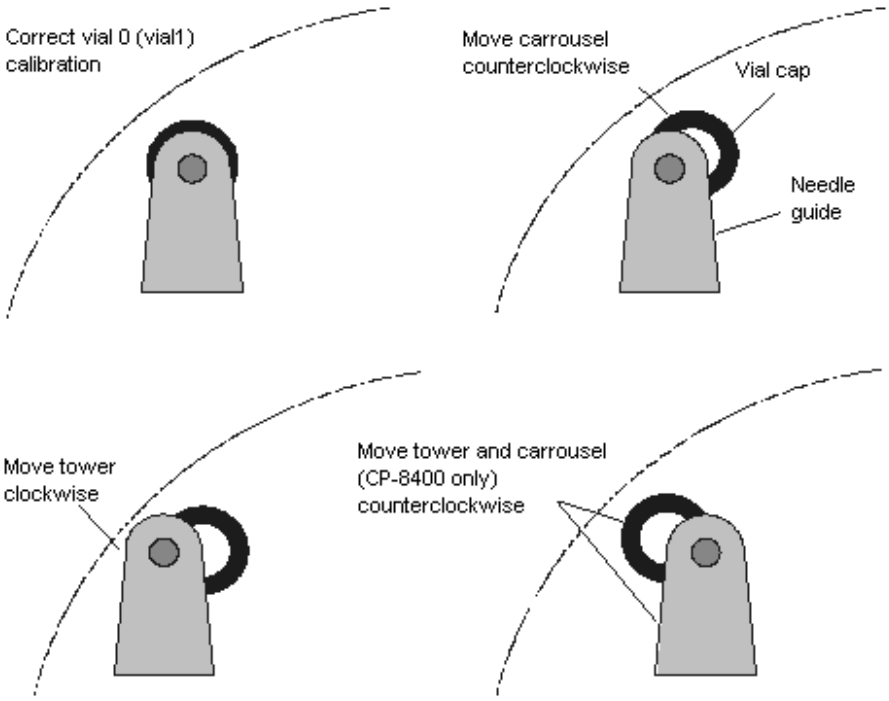
   Calibrating the vial 0 (or vial 1 if 8410) position involves manipulating the positions of three different components. The object of the calibration is to position the needle as closely as possible over the center of the sampling target area of the vial. Upon starting the calibration procedure, the 8400/8410 will rotate the tower, rotate the carousel (on the 8400 only), and lower the syringe sled to the approximate location of vial 0 (or vial 1).

3. After the 8400/8410 has found the approximate vial 0 (or vial 1) position and before going further, visually check that the syringe sled is not resting on the vial top. If it is, use the following buttons, in the *Moving Tower / Syringe* section, to move the sled so that the needle guide is approximately 1 mm above the vial:

   to move the syringe up.

   to move the syringe down.

4. Start the calibration process by adjusting the tower position as shown below:



Tower Position Calibration

5. Use the following buttons, in the *Moving Tower / Syringe* section, to adjust tower position:

   to move the tower 1 step in the clockwise direction each time the button is pressed.

   to move the tower 10 steps in the counterclockwise direction each time the button is pressed.

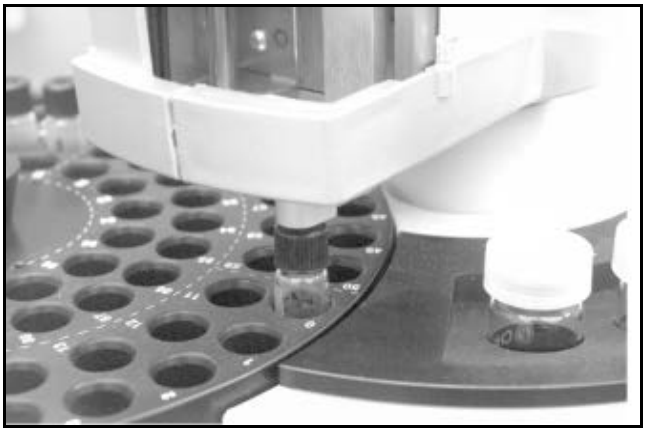
6. Next, for 8400 users only, set the carousel position. Use the following buttons, in the *Moving Carousel* section, to adjust carousel position:

   to move the carousel 1 step in the clockwise direction each time the button is pressed.

   to move the carousel 10 steps in the counterclockwise direction each time the button is pressed.

7. Finally, adjust the Syringe sled height so that the needle guide is just barely above the vial cap. You should be able to see about a paper thickness of space between the needle guide and the top of the vial cap. The penetration depth into the vial is measured from the bottom of the needle guide, so this height will give you optimum penetration depth.

When the Vial 0/Vial 1 calibration is correctly set, the needle guide should be positioned over the vial top as shown below.



Correct Vial Calibration

Press the Save Calibration (F2) button (or the F2 key) in the Calibrate Vial 0 (or 1) Position field, to complete the calibration of the vial or press the button to cancel calibration: the autosampler will recover its initial position.

Injector Calibration:

After completing the vial position calibration you will need to calibrate the injector position.

1. Press the Start Calibration (F3) button (or the F3 key) in the *Calibrate Injector Position* field.

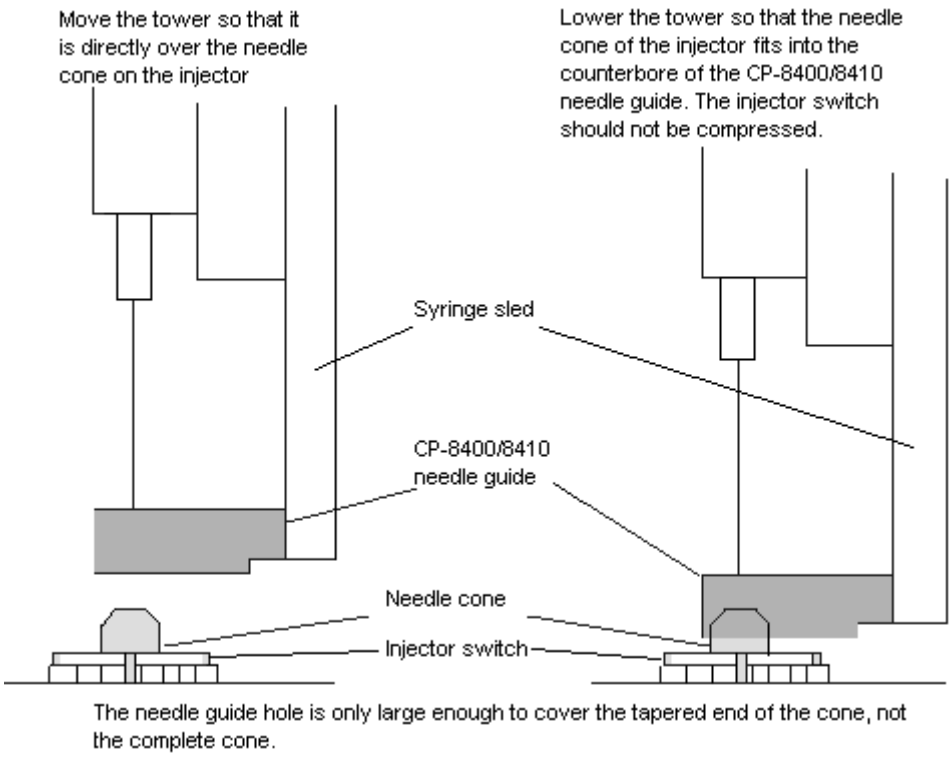
   The syringe tower will rotate so that it is approximately over the injector and the syringe sled will descend to a point near the top of the injector.

Use the following buttons, in the Moving Tower / Syringe section, to adjust the syringe position:

to move the syringe up.

to move the syringe down.

The needle guide should just cover but not depress the cone on the inject switch as shown below:


Move the tower so that it is directly over the needle cone on the injector
Lower the tower so that the needle cone of the injector fits into the counterbore of the CP-8400/8410 needle guide. The injector switch should not be compressed.
Syringe sled
CP-8400/8410 needle guide
Needle cone
Injector switch
The needle guide hole is only large enough to cover the tapered end of the cone, not the complete cone.

Correct Syringe Sled / Injector Position

2. Move the tower so that it is directly over the needle cone on the injector. Lower the tower so that the needle cone of the injector fits into the counter bore of the 8400/8410 needle guide.

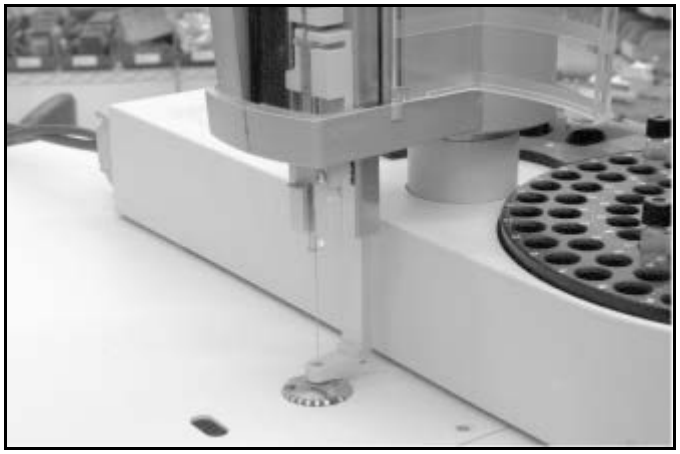
Use the following buttons, in the Moving Tower/Syringe section, to adjust tower position:

to move the tower 1 step in the clockwise direction each time the button is pressed.

to move the tower 10 steps in the counterclockwise direction each time the button is pressed.

NOTE: The injector switch should not be compressed. If the injector switch is compressed, you may experience ‘syringe sled’ errors during autosampler operation. If you are uncertain whether the inject switch is compressing, it is better to raise the syringe sled 1 or 2 steps.

When you have completed the tower and sled movements, the system should look as in the figure below:



Correct Injector Calibration

3. Press the Save Calibration (F4) button (or the F4 key) in the *Calibrate Injector Position* field, to complete the calibration of the injector or press the button to cancel calibration: the autosampler will recover its initial position.

4. Press the Done button to exit the autosampler calibration screen.

Using the keyboard to adjust positions

The positions of the tower, the syringe or the carousel can also be adjusted by using the following keys:

Tower / Syringe movement

equivalent to the up arrow key.

equivalent to the down arrow key.

equivalent to the left arrow key.

equivalent to the right arrow key.

equivalent to the home key.

Carousel movement

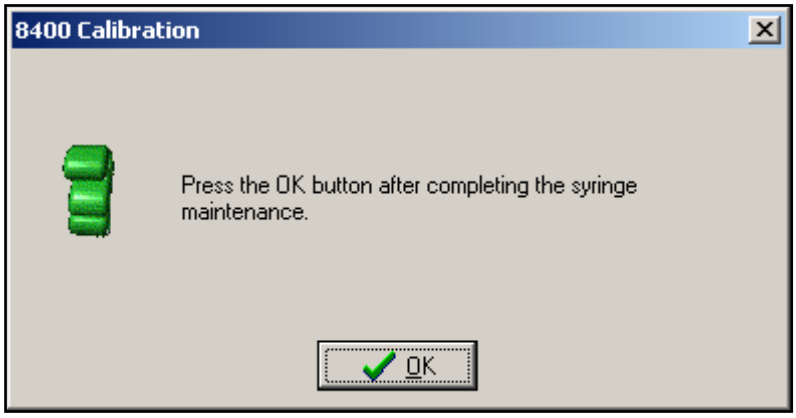
equivalent to the page up key.

equivalent to the page down key.

Syringe Maintenance

1. Press the Change Syringe (F5) button (or the F5 key): the tower will rotate so as you will have easy access to the syringe (for routine service, syringe removal and replacement…). The buzzer will sound before any tower movement occurs.

2. When the syringe has been changed, press the *OK* button in the following message screen:



3. The tower will return to its previous position and state. The buzzer will sound prior to movement as designated by the Buzzer on Start Cycle setting.

4. Press the Clear Plunger Count (F6) button (or the F6 key) to reset the plunger stroke count to 0. The following warning message appears:

Validate or cancel the operation by clicking on Yes or No.

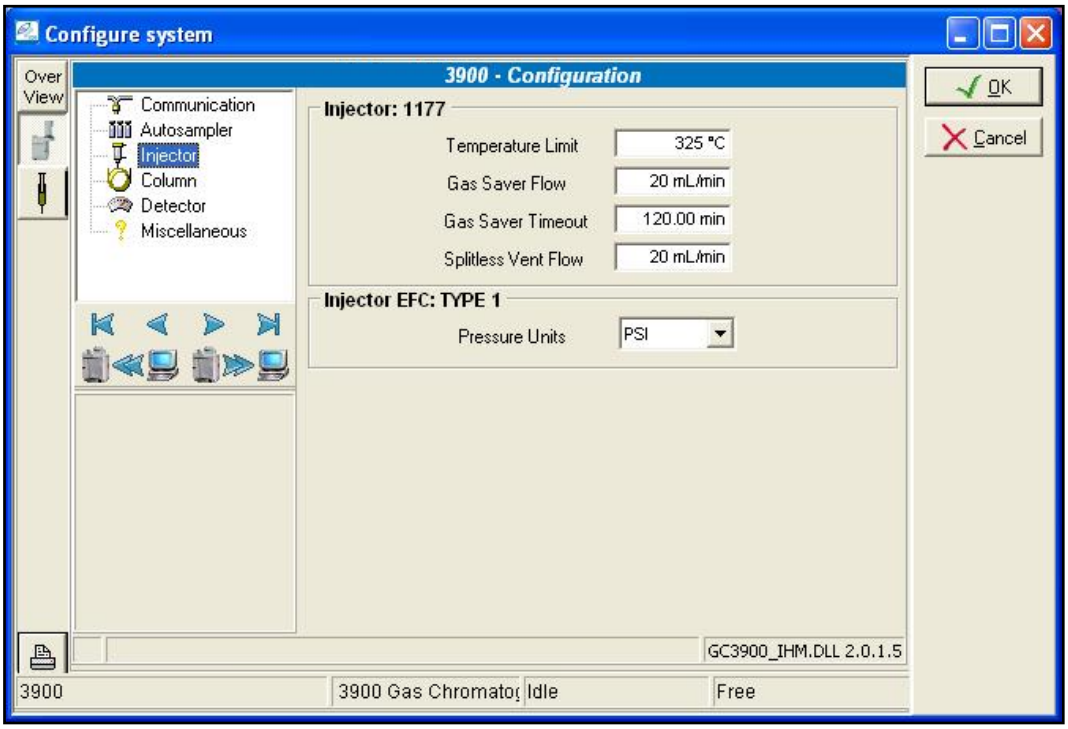
5. Press the Done button to exit the autosampler calibration screen.

Injector Window

1177 Injector

According to the 3900 GC model (with or without a keypad), information in this screen is different.

In case of a chromatograph with a keypad, the following screen is displayed:



Injector Parameter Group

Enter the upper temperature limit of the injector in the Temperature Limit field (50 to 450 °C).

Enter the lowest system flow rate that will be maintained during the gas saver period in the Gas Saver Flow field (1 to 100 mL/min, default = 20).

Enter the Gas Saver Timeout in the corresponding field [0 (Off) to 999.99 min]. A non-zero value entered for this parameter will cause the system to initiate a timer once a method is activated. If no system actions such as a run start or another method activation occurs before the gas saver timeout is reached, then the system will reduce the flow through the system to the gas saver flow. A method activation action will clear the gas saver flow and bring the system to Ready for subsequent injections.

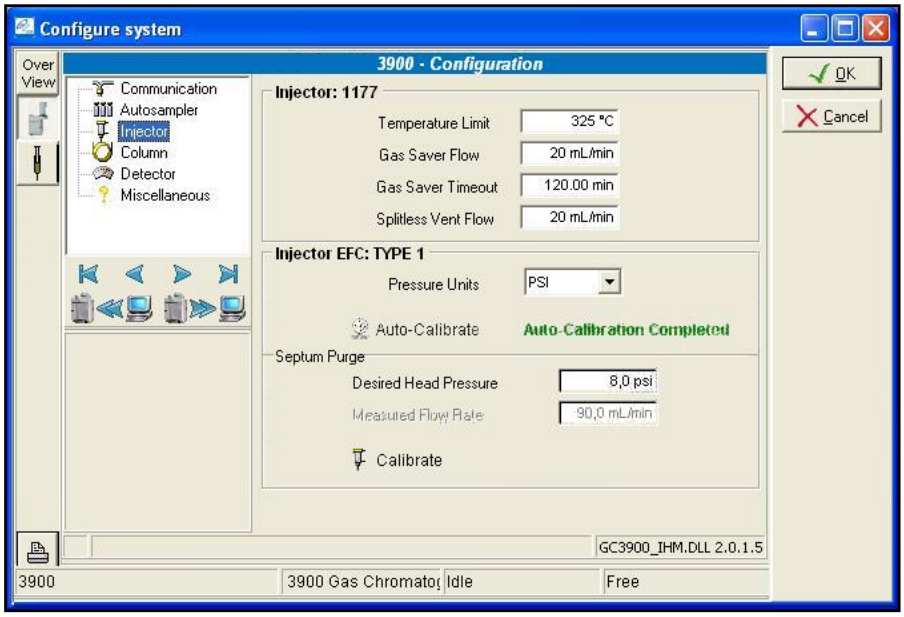
A zero value entered for the gas saver timeout will cause the gas saver flow to be ignored and no gas saver actions will be performed.

Define the Splitless Vent Flow (0 to 500 mL/min) which corresponds to the flow the system will vent when the split valve is left closed for the duration of the run. This flow is diverted before the injector and thus does not influence the splitless nature of the run. This entry is ignored during split and splitless runs in which the split vent is opened.

Injector EFC Type 1 Parameter Group

Select from the list the Pressure Units of the injector EFC (Electronic Flow Control). Three choices are available: PSI, kPa, Bar.

In case of a chromatograph without a keypad, the following screen is displayed:



Parameters are the same that for a chromatograph with a keypad, plus an Auto-Calibrate button and a Septum Purge part.

Click on the Auto-Calibrate button to automatically calibrate the EFC system.

When it is finished, a successful completion or detected problem message is displayed.

No other GC functions can be performed during Autocalibration.

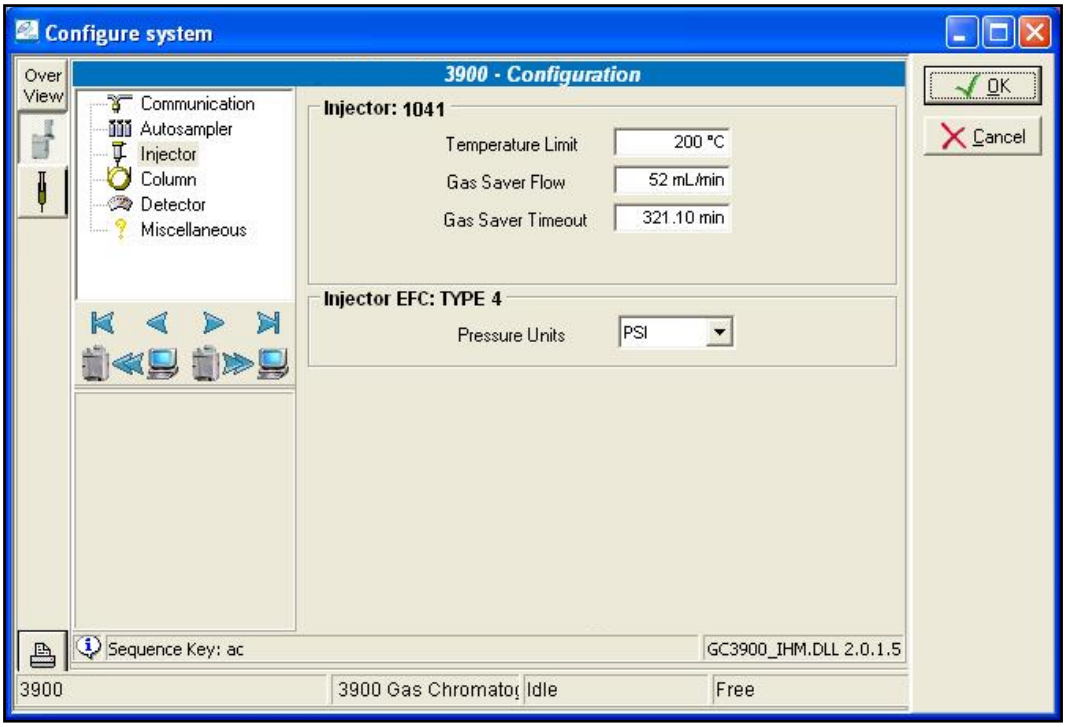
To calibrate the Septum Purge flow, perform the following steps:

1. Type the pressure in the Desired Head Pressure field.
2. Click on the Calibrate button.
3. Using a flow meter, measure the septum purge flow rate and type it in the Measured Flow Rate field.
4. Click on the Calibrate button.

NOTE: After installing a new column, the septum purge should be calibrated.

NOTE: The septum purge flow rate is adjustable but is typically set at 3-5 mL/min.

1041 Injector



Injector Parameter Group

Enter the upper temperature limit of the injector in the Temperature Limit field (50 to 450 °C).

Enter the lowest system flow rate that will be maintained during the gas saver period in the Gas Saver Flow field (1 to 100 mL/min, default = 20).

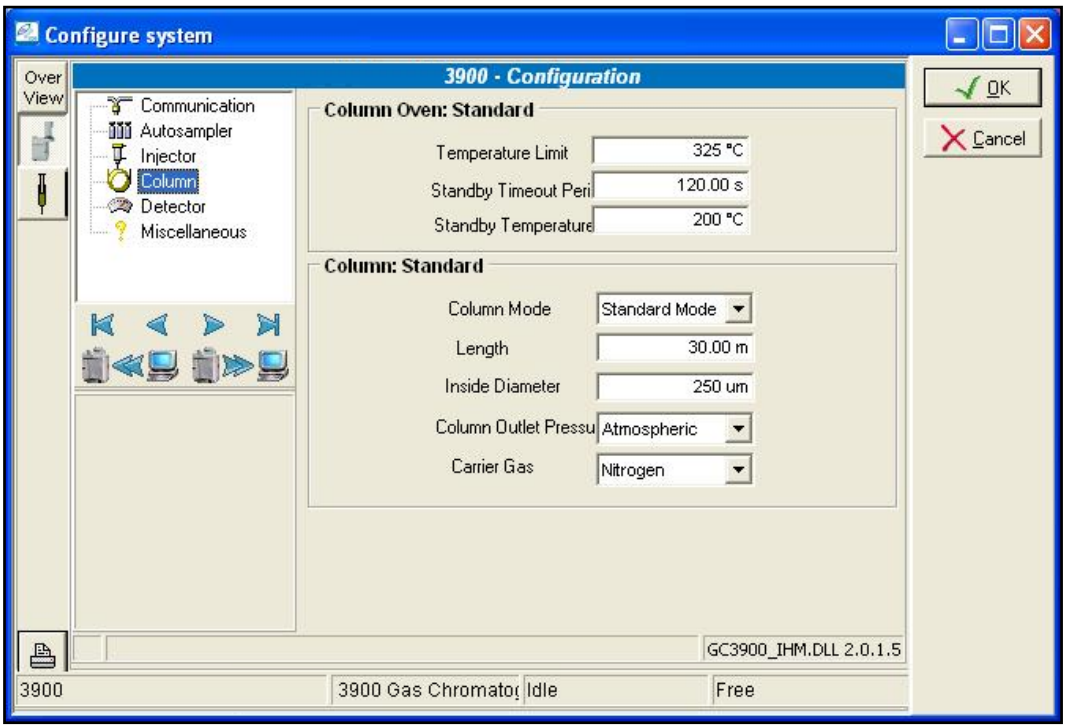
Enter the Gas Saver Timeout in the corresponding field (0 -Off- to 999.99 min). A non-zero value entered for this parameter will cause the system to initiate a timer once a method is activated. If no system actions such as a run start or another method activation occurs before the gas saver timeout is reached, then the system will reduce the flow through the system to the gas saver flow. A method activation action will clear the gas saver flow and bring the system to Ready for subsequent injections.

A zero value entered for the gas saver timeout will cause the gas saver flow to be ignored and no gas saver actions will be performed.

Injector EFC Type 4 Parameter Group

Select from the list the Pressure Units of the injector EFC (Electronic Flow Control). Three choices are available: Psi, kPa, bar.

Column Window



Column Oven Parameter Group

Enter the upper Temperature Limit of the column oven in the corresponding field (50 to 450 °C).

Enter the Standby Timeout Period in the corresponding field (0 to 999 min).

Enter the Standby Temperature in the corresponding field (30 to 250°C).

When the Column Standby Temperature is enabled, the GC will be held Not Ready until Reset is pressed on the instrument or the Standby Temperature is disabled.

Column Parameter Group

Select the required Column Mode. Two choices are proposed: Standard Mode (by default) or Rapid MS Mode. Rapid MS Mode is only applicable to a Rapid MS column used in a 2100 GC/MS system.

Enter the column Length (0 to 250 m) and Inside Diameter (0 to 999 µm) in the corresponding fields.

Select from the list the Column Outlet Pressure (Atmospheric or Vacuum – for MS detectors).

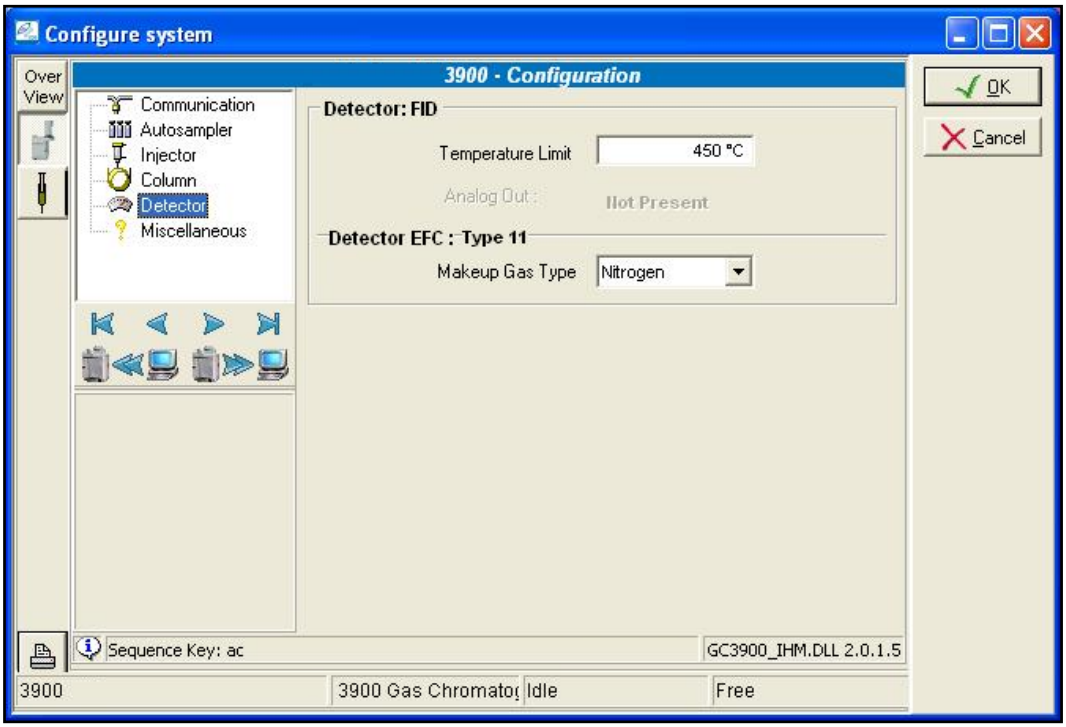
Select the Carrier Gas from the list. The following choices are available: Helium, Hydrogen, and Nitrogen.

Detector Window

FID Detector

According to the 3900 GC model (with or without a keypad), information in this screen is different:

In case of a chromatograph with a keypad, the following screen is displayed:



Detector Parameter Group

Enter the upper Temperature Limit of the detector in the corresponding field (50 to 450 °C).

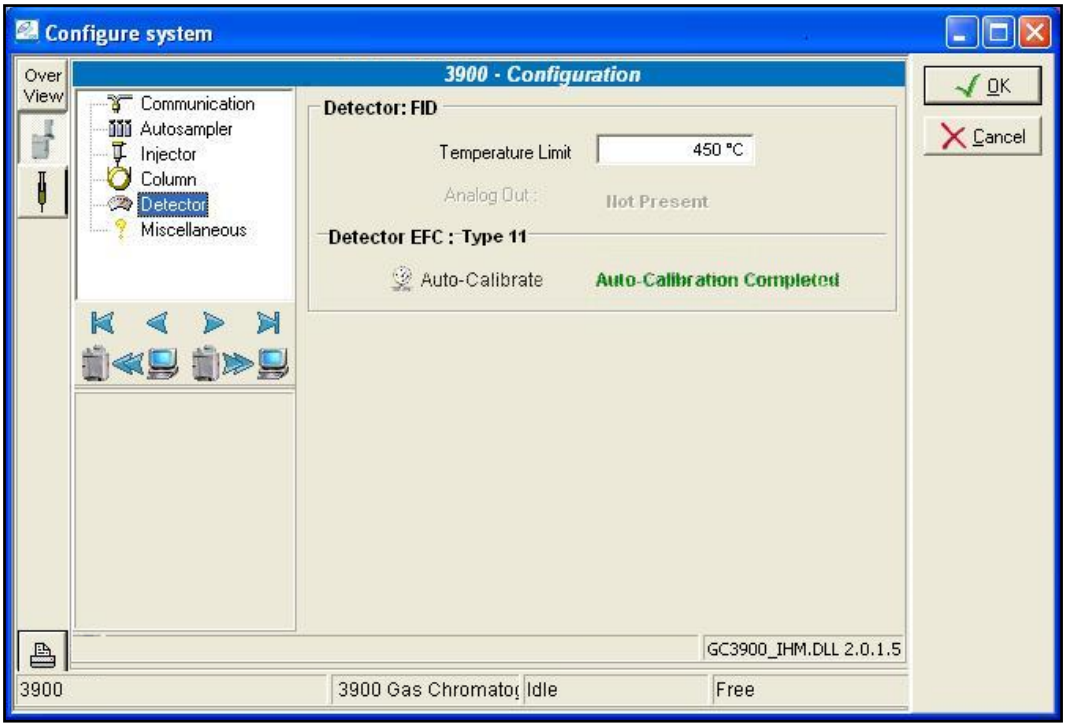
If the Analog Output is configured on the GC, the corresponding field is active and Present is displayed.

Detector EFC Parameter

For FID detectors, the EFC Type 11 is required.

Select the Makeup Gas Type from the list. Three choices are available: Helium, Nitrogen and Argon.

In case of a chromatograph without a keypad, the following screen is displayed:



Parameters are the same that for a chromatograph with a keypad, plus an Auto-Calibrate button.

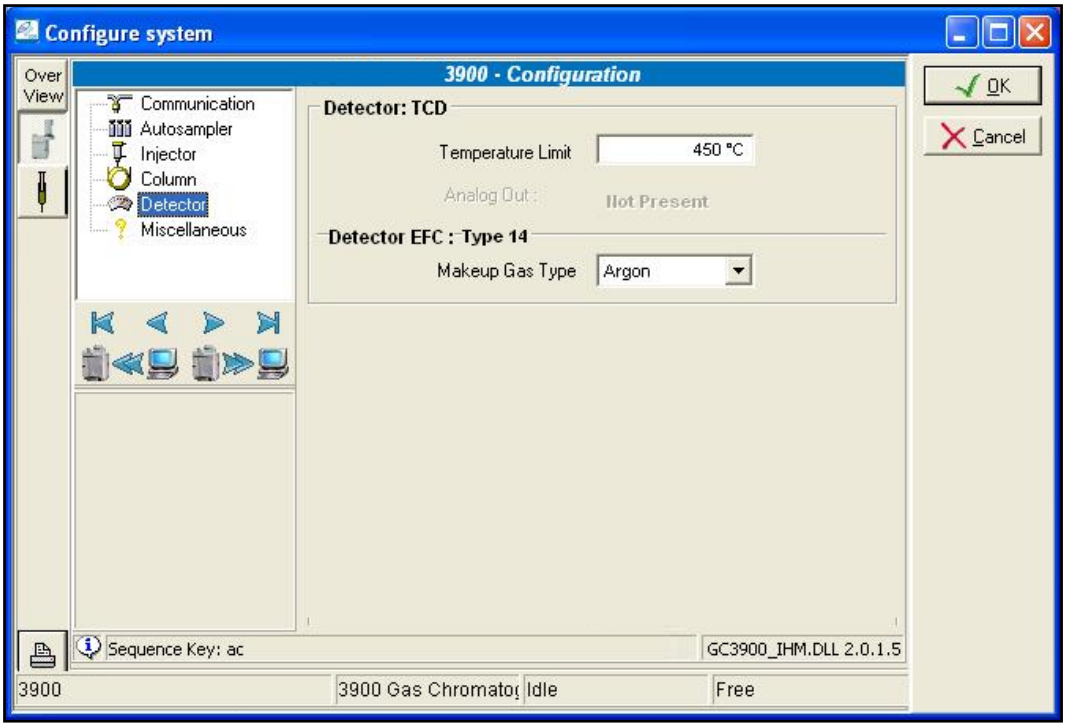
Click on the Auto-Calibrate button to automatically calibrate the EFC system.

When it is finished, a successful completion or detected problem message is displayed.

No other GC functions can be performed during Autocalibration.

NOTE: Autocalibration should be done on a semiannual basis.

TCD Detector



Detector Parameter Group

Enter the upper Temperature Limit of the detector in the corresponding field (50 to 450 °C).

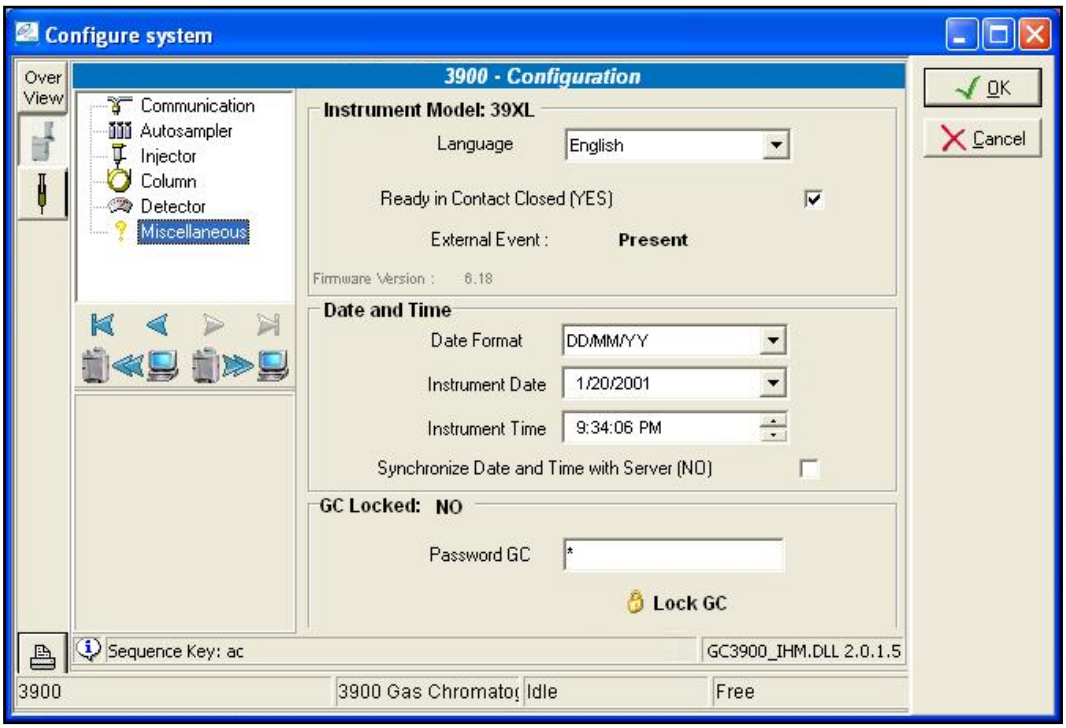
If the Analog Output is configured on the GC, the corresponding field is active and Present is displayed.

Detector EFC Parameter

For TCD detectors, the EFC type 14 is required.

Select the Makeup Gas Type from the list. Three choices are available: Helium, Nitrogen and Argon.

Miscellaneous Window



Instrument Model Parameter Group

Select the Language of the instrument. Here are the available choices: English, French, Italian, Spanish, German, Katakana (Japanese).

The Ready in Contact Closed option allows you to specify what switch state corresponds to external device Ready. Check the option if the closed state means Ready.

The presence of External Events is also displayed in this screen.

Date and Time Parameter Group

This section allows you to select the Date Format (MM/DD/YY or DD/MM/YY), the Instrument Date and Instrument Time and to choose whether or not to synchronize GC date and time with the server.

GC Locked Parameter Group

To lock or unlock the GC type the password in the password GC field and press the button Lock GC or Unlock GC.

If the GC is locked by a password before CompassCDS takes control of the GC, no method can be downloaded in the GC if the password is not specified in the password GC field.

Configuring the Synopsis

In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

To save the configuration of these devices, click on the OK button.

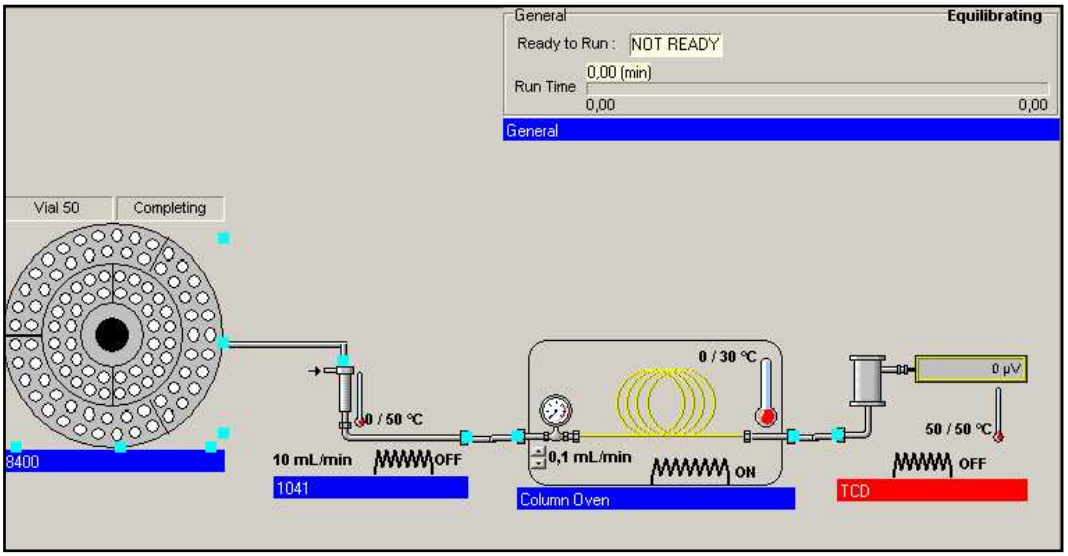
Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

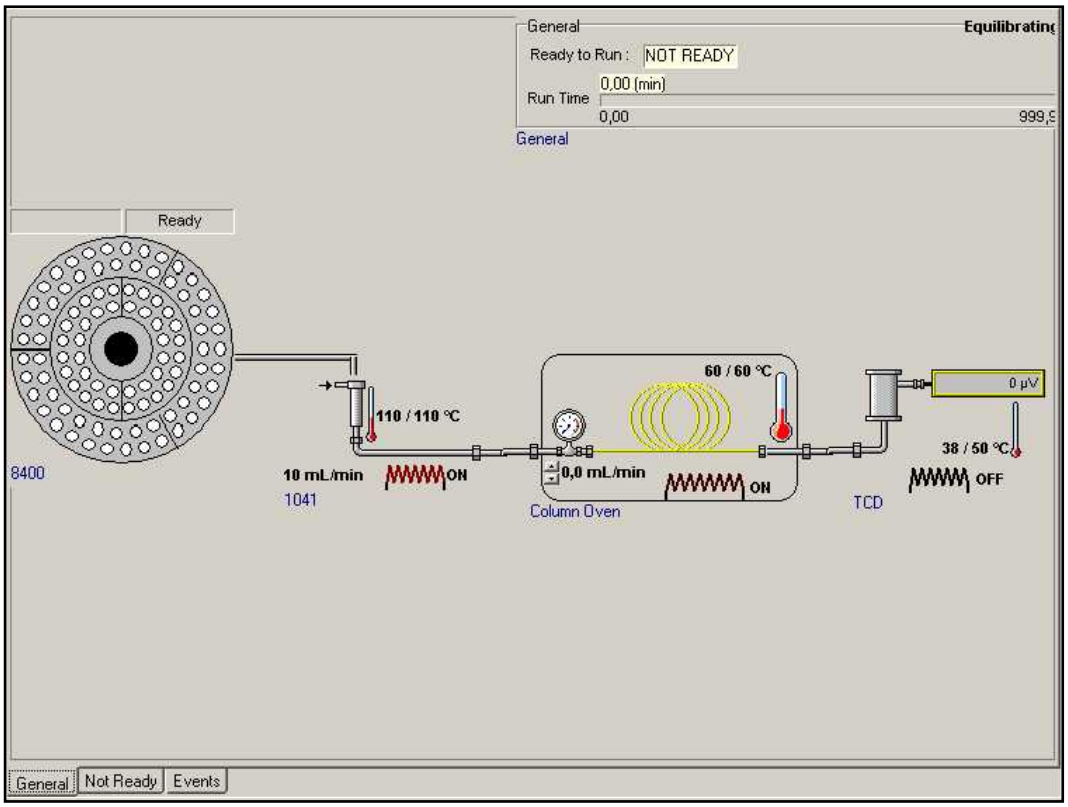
Go back to the System Configuration screen (Properties wizard). A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, then connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

Click on the to delete a selected tube; click on the button to delete all the tubes.
Click on to define a background color, or on to make the background transparent.
Click on the icon to change the grid color.

Once the synopsis configuration is complete, it will be displayed in CompassCDS, in the Systems tab. In this tab, the Overview will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.), depending on the installed devices.

For example, the following pictures represent the synopsis of the 3900 GC:





NOTE: Once the system has been created and correctly configured, it must be associated to one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current 3900 GC configuration.

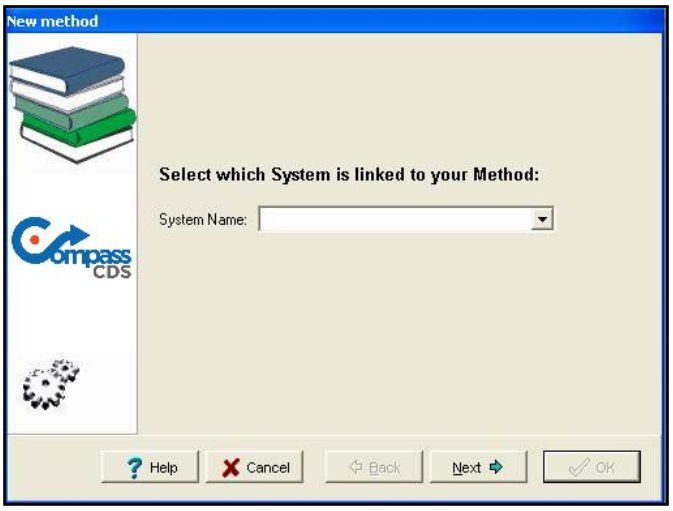
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

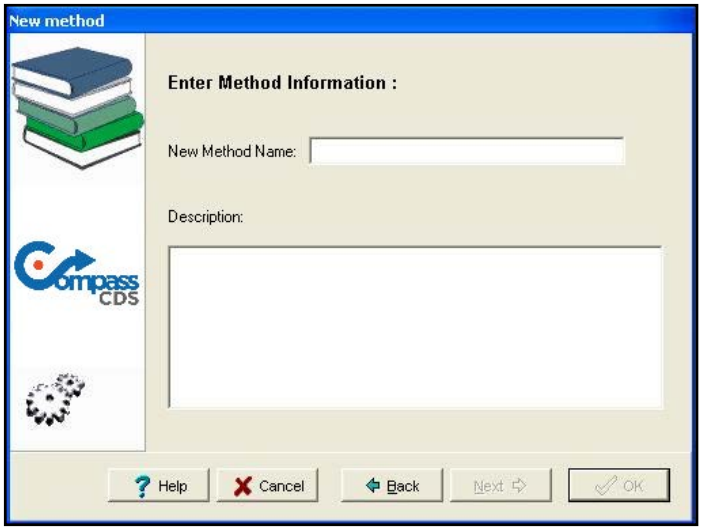
To create a new method, select the FILE / NEW METHOD option from CompassCDS main menu.

A wizard guide will appear and provide assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

Once this field is completed, click on the Next button to move to the second step of the method creation:



Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

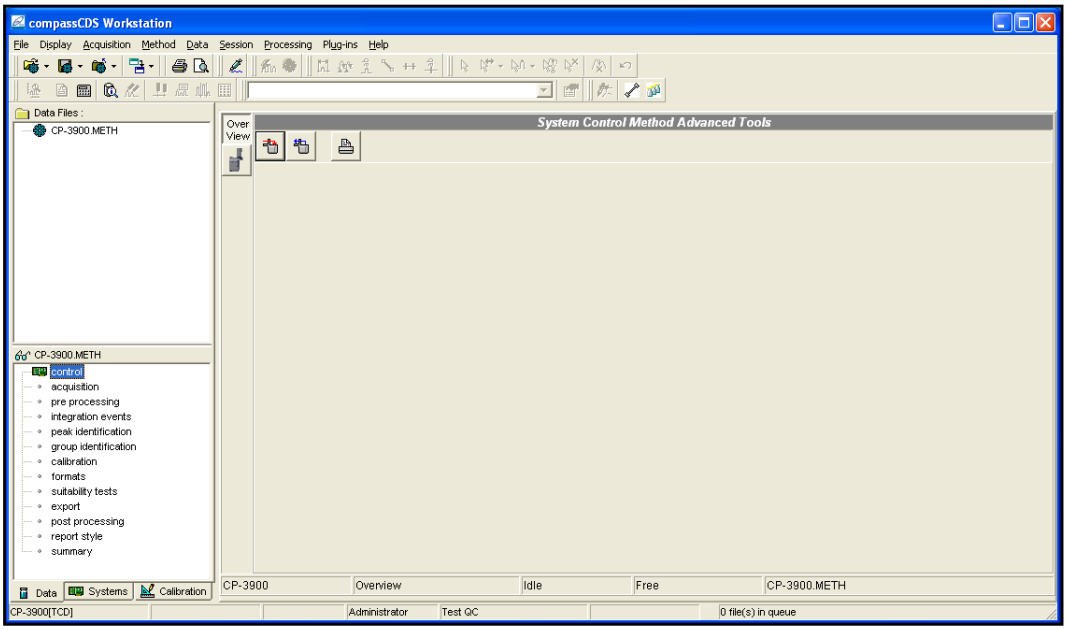
The instrument control section must be defined to start an acquisition. In the following part of this guide, only the control section of the method for the 3900 GC is detailed. Other parameters such as Injection Volume, Vial, and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, refer to CompassCDS User Guide.

Control Method Section for the 3900 GC

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



Press the Over View button to display the System Control Method Advanced Tools window:

to send the current method to the instrument

to get the active method from the instrument

to print the current method

Click on the button to display the 3900 control method section. It contains seven sub-sections: Autosampler, Injector, Oven, Column Pneumatics, Detector, External Events, and Miscellaneous. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

The toolbar allows you to easily scroll through the control method windows:

to select the first window of the control method.

to select the first window of the control method.

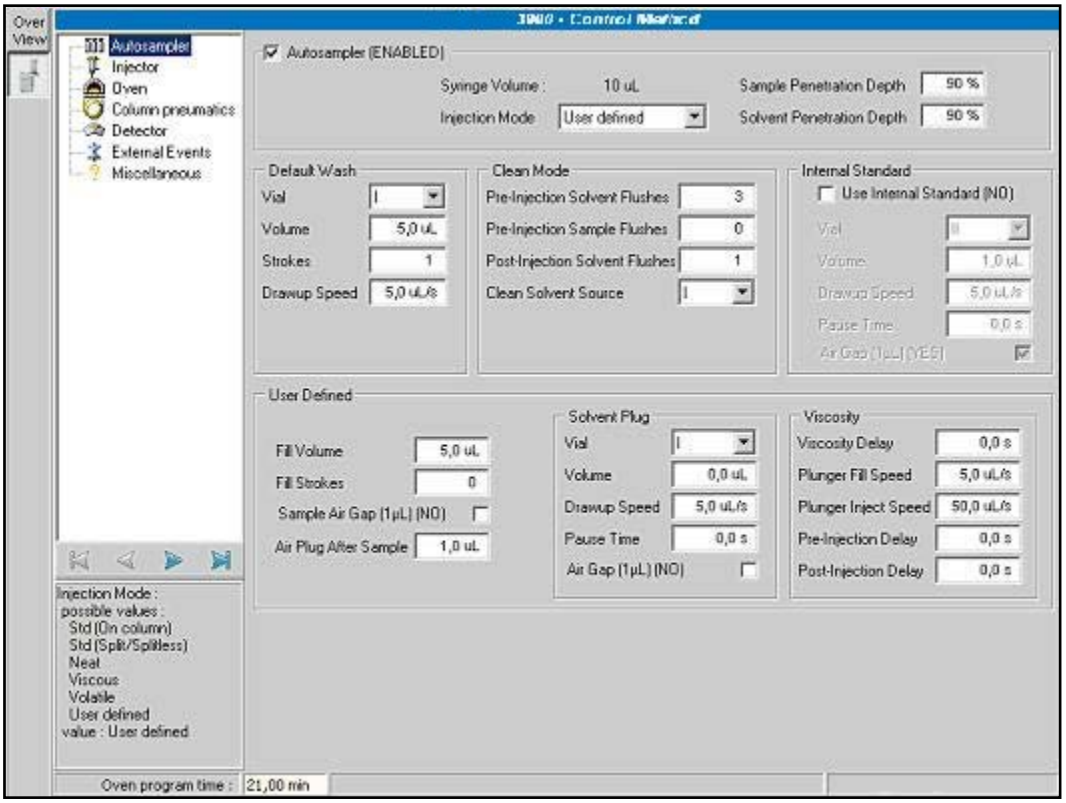
to select the first window of the control method.

to select the final window of the control method.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Autosampler Control

The autosampler window contains sampling parameters for the 8400/8410 Autosampler when attached to the 3900 GC:



Autosampler Parameter Group

In this parameter group, define the sampling syringe size (Syringe Volume), the Injection Mode and the Penetration Depth for sample and solvent wash vials.

Parameter	Description
Autosampler	When unchecked, this option allows you to inject manually and to not use the autosampler (when unchecked, all the sampler parameters become non-active).
Syringe Volume (µL)	Selects the size of the syringe that is installed on the instrument.
Injection Mode	Consists of five predefined injection modes: Standard Split/Splitless, Standard On-Column, Neat, Viscous and Volatile. A sixth User Defined mode is available and allows you access to all autosampler parameters to fine-tune your injection.
Sample Penetration Depth (%)	Specifies how far the syringe needle is to go down into the sample vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.
Solvent Penetration Depth (%)	Specifies how far the syringe needle is to go down into the solvent vial. 100% corresponds to the bottom of the vial. 0% is the bottom of the vial septum.

NOTE:

The *standard* mode is the default and typically yields good results in most applications.

The *volatile* sampling mode is used for sampling solvents with high vapor pressures at room temperature.

The *neat sampling* mode is used for pure samples requiring minimum contamination with wash solvent (this mode does not use a solvent plug).

The *viscous sampling* mode is used for samples with a higher viscosity than water.

Default Wash Parameter Group

In the Default Wash fields, define the parameters that will be used during the default cleaning which is used in case automation is stopped or a serious fault is detected.

Parameter	Description
Vial	Specifies which of the three solvent vials will be used by the default cleaning.
Volume (µL)	Specifies the amount of cleaning solvent that will be drawn up with each syringe cleaning stroke.
Strokes	Specifies the number of times the cleaning solvent will be drawn up into the syringe and expelled into the waste cup.
Drawup Speed (µL/s)	Specifies speed at which the cleaning solvent will be drawn up into the syringe and the speed at which it is expelled into the waste cup.

Clean Mode Parameter Group

In the Clean Mode fields, define the pre and post injection syringe clean modes.

Parameter	Description
Pre-Injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified) or the sample, before injection.
Pre-Injection Sample Flushes	Specifies the number of times the sample will be drawn up into the syringe and expelled into the waste cup before the syringe is loaded for injection.
Post-Injection Solvent Flushes	Specifies the number of times each selected cleaning solvent will be drawn up into the syringe and expelled into the waste cup before flushing with next cleaning solvent (if more than one cleaning solvent source is specified), after injection.
Clean Solvent Source	Selects which solvent vial or sequence of solvent vials will be used to flush the syringe before and after injection.

Internal Standard Parameter Group

The Internal Standard section is displayed when one of the following injection modes is selected: Viscous, Volatile or User-defined.

If the Use Internal Standard option is checked, an internal standard solution will be drawn up into the syringe from the specified solvent vial before the sample is drawn up.

Parameter	Description
Vial	Selects which solvent vial contains the internal standard.
Volume (µL)	Specifies the amount of internal standard to be drawn into the syringe before the sample.
Drawup Speed (µL/s)	Specifies the speed at which the internal standard will be drawn up into the syringe.
Pause Time	Defines how long the syringe is to remain in the internal standard vial after drawing up the internal standard.
Air Gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap between the internal standard and the sample

NOTE: When this mode of injection is selected, beware that the total volume (volume of sample injected, entered in the Volume field of the Acquisition method section + Volume of internal standard + volume of any air gaps) does not exceed the maximum syringe volume or the autosampler will be faulted and the GC will stay in the Waiting for injection state.

User Defined Parameter Group

When the User Defined injection mode has been selected, another parameter group is displayed and allows you to define the general, Solvent Plug and Viscosity parameters:

User Defined Parameters

Parameter	Description
Fill Volume (µL)	Specifies the sample volume that will be used for each fill stroke.
Fill Strokes	Specifies the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.
Sample Air Gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the sample plug.
Air Plug After Sample	Specifies the volume of room air that will be drawn into the syringe after it is loaded with sample.

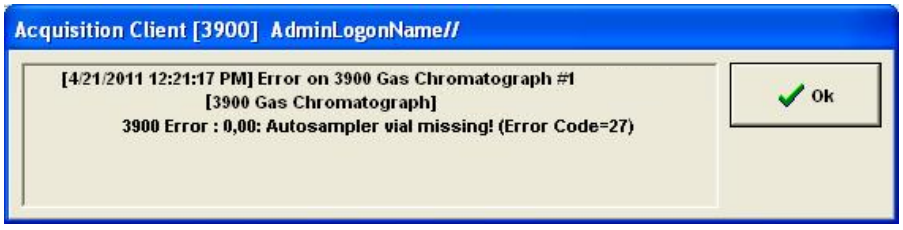
Solvent Plug Parameters

Parameter	Description
Vial	Selects which solvent vial to use for the solvent plug.
Volume (µL)	Specifies the amount of solvent to be drawn into the syringe before the sample or internal standard.
Drawup Speed (µL/s)	Specifies the speed at which the solvent will be drawn up into the syringe.
Pause Time	Defines how long the syringe is to remain in the solvent vial after drawing up the solvent.
Air Gap	When the option is checked, 1 µL of room air will be drawn into the syringe to create an air gap before the solvent plug.

Viscosity Parameters

Parameter	Description
Viscosity Delay (sec)	Specifies how long the syringe is to remain in the sample vial after drawing up the sample.
Plunger Fill Speed (µL/sec)	Specifies the speed at which the sample will be drawn up into the syringe.
Plunger Inject Speed (µL/sec)	Specifies the speed at which the contents of the syringe will be expelled into the injector.
Pre-Injection Delay (sec)	Specifies the length of time the syringe needle resides in the injector before expelling the syringe contents.
Post-Injection Delay (sec)	Specifies the length of time the syringe needle remains in the injector after expelling the syringe contents.

NOTE: When a vial is missing, the following message appears and you have 10 minutes to replace the sample in the correct vial position before the system skips the missing vial and passes to the next line of the sequence or stops the run. When you have replaced the missing sample, you must go to the *Systems* tab, click on the instrument icon, select the *Miscellaneous* tab and click on the Re-inject button to restart the run. If you want to skip the missing vial and start the next run, you must press the Skip vial button.


Acquisition Client [3900] AdminLogonName//
[4/21/2011 12:21:17 PM] Error on 3900 Gas Chromatograph #1
[3900 Gas Chromatograph]
3900 Error : 0,00: Autosampler vial missing! (Error Code=27)
Ok

Warning Message When a Vial is Missing.

Default Settings for Predefined Autosampler Mode

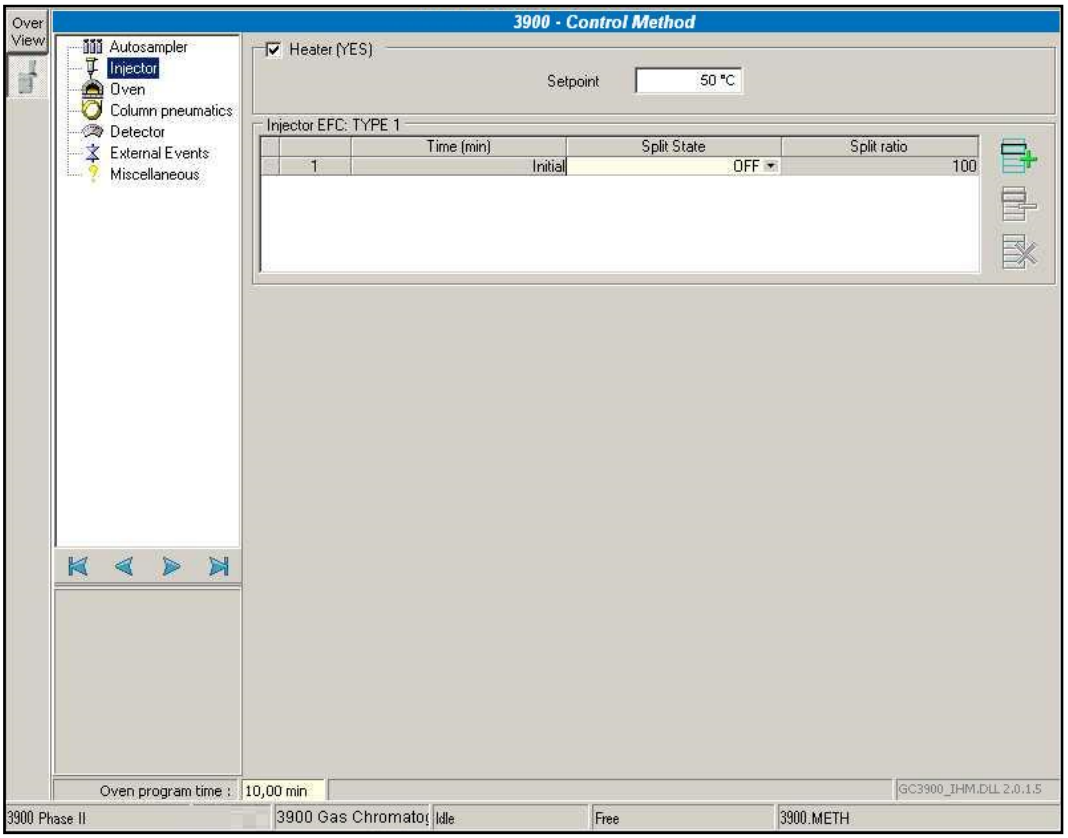
The following table lists the parameter settings used for each of the Predefined 8400/8410 modes using a 10 microliter syringe. If the predefined modes do not work acceptably for your samples, use the User Defined mode to enter settings that will work better with your samples. The values listed in this table provide a starting point for setting the various parameters.

Parameter	Std Split/ Splitless	Std On-Column	Neat*	Volatile	Viscous
Solvent Plug Settings:	Solvent plug is not used with predefined modes. If you wish to use solvent plug injections, you must use User Defined mode.				
Predefined Settings:					
Fill Volume	7.5 µL	7.5 µL	Not used	Not used	Not used
Fill Strokes	5	5	0 [1]	0	0
Sample Air Gap	No	No	No	No	No
	1 µL	1 µL	1 µL	1 µL	1 µL
Viscosity Settings:					
Delay	0 sec	0 sec	0 sec	6 sec	9.9 sec
Fill Speed	2 µL/sec	2 µL/sec	2 µL/sec	1 µL/sec	1 µL/sec
Inject Speed	50 µL/sec	2 µL/sec	50 µL/sec	1 µL/sec	5 µL/sec
Air Plug After Sample	0 sec	0 sec	0 sec	0 sec	0 sec
Post-Injection Delay	0 sec	6 sec	0 sec	0 sec	12 sec

[1] Instead of fill strokes, Neat mode fills the syringe with sample at 2 µL/sec then expels it into the waste cup at 50 µL/sec. It does this a total of six times. Then it fills the syringe with sample at 2 µL/sec and expels it back into the sample vial at 50 µL/sec. This “pumping” action is done three times. After this is completed, the sample is loaded into the syringe and injected using the parameters in the table.

Injector Control

1177 Injector



Check or uncheck the Heater option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the Setpoint field (50 to 450 °C).

Injector EFC Parameter Group

If the injector is connected to a Type 1 EFC, you can build a split ratio time program by using the split event table:

The first row of the spreadsheet contains the Initial Split State and Split Ratio for the injector. The injector will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed.

The rest of the spreadsheet contains the time-programmed settings for the injector Split Ratio: The Split Valve will be switched to the ratio in each row at the indicated time. If the Split State is ON, then the sample is split according to the Split Ratio specified in the corresponding column. If the state is OFF, the entire sample enters the column.

The split ratio is defined as the column flow plus the split flow, divided by the column flow.

NOTE: You must have already configured the Type 1 EFC in the configuration manager (CompassCDS Configuration Manager) before you can program the split ratio. You can use a split ratio of 100 after injection to vent the injector of any residual solvent. Use a very low split ratio after flushing to conserve carrier gas.

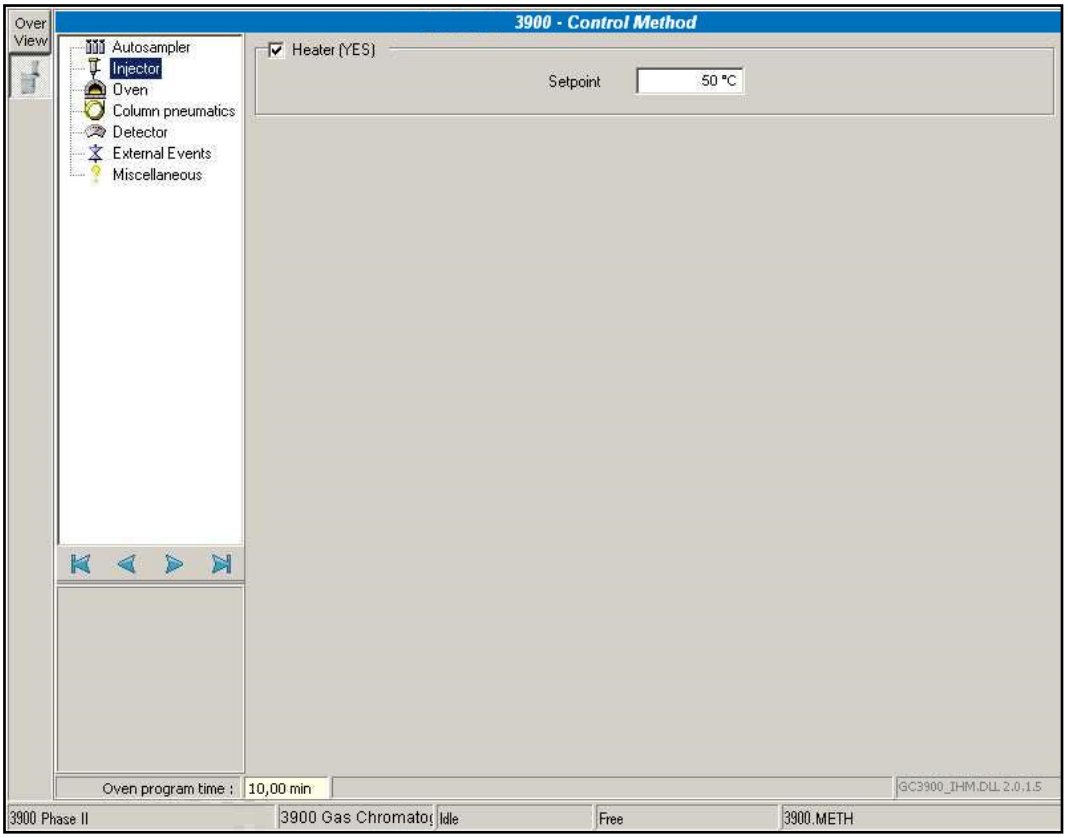
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

1041 Injector

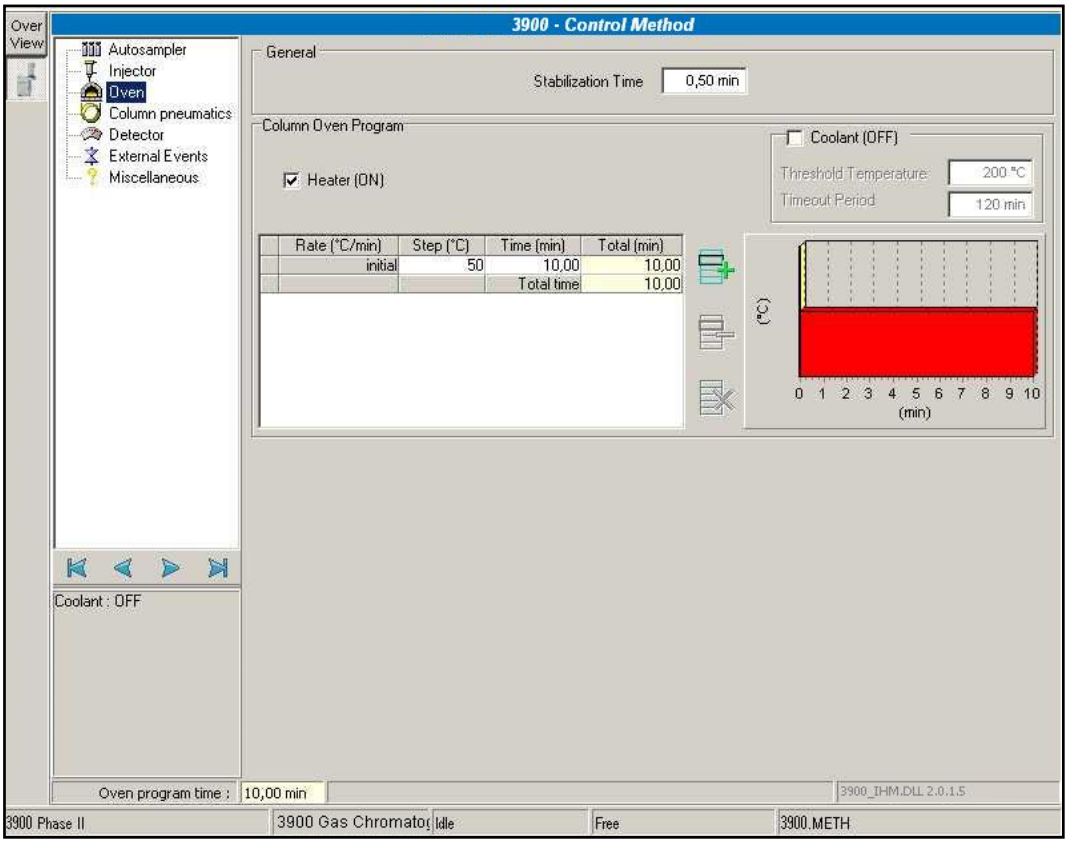


Check or uncheck the Heater option to turn the injector oven ON or OFF.

Enter the injector oven temperature in the Setpoint field (50 to 450 °C).

Column Oven Control

The Column oven window contains the column oven program:



General Parameter

Enter the Stabilization Time in the corresponding field (0.00 to 10.00 min).

Column Oven Program Parameter Group

Check or uncheck the Heater option to turn it ON or OFF.

Use the spreadsheet to build a temperature ramp program to heat and/or cool the column oven.

The first row of the spreadsheet contains the Initial temperature and hold time for the column oven. The column oven will equilibrate to this setting and stabilize for the specified Stabilization Time (defined in the General field), when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the programmed settings for each of the ramp segments. Enter the final temperature of each ramp segment in the Step column (30 to 450 °C), the Rate (0.1 to 100.0 °C/min) and the Time (0.00 to 999.99 min) the column oven is held at this temperature in the corresponding columns.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

The graph shows the column oven temperature program.

Check the Coolant option if you want to turn the column coolant valve ON. Specify the temperature for the coolant valve to turn on in the Threshold Temperature field (50 to 250°C) and the Timeout Period (0 to 999 min).

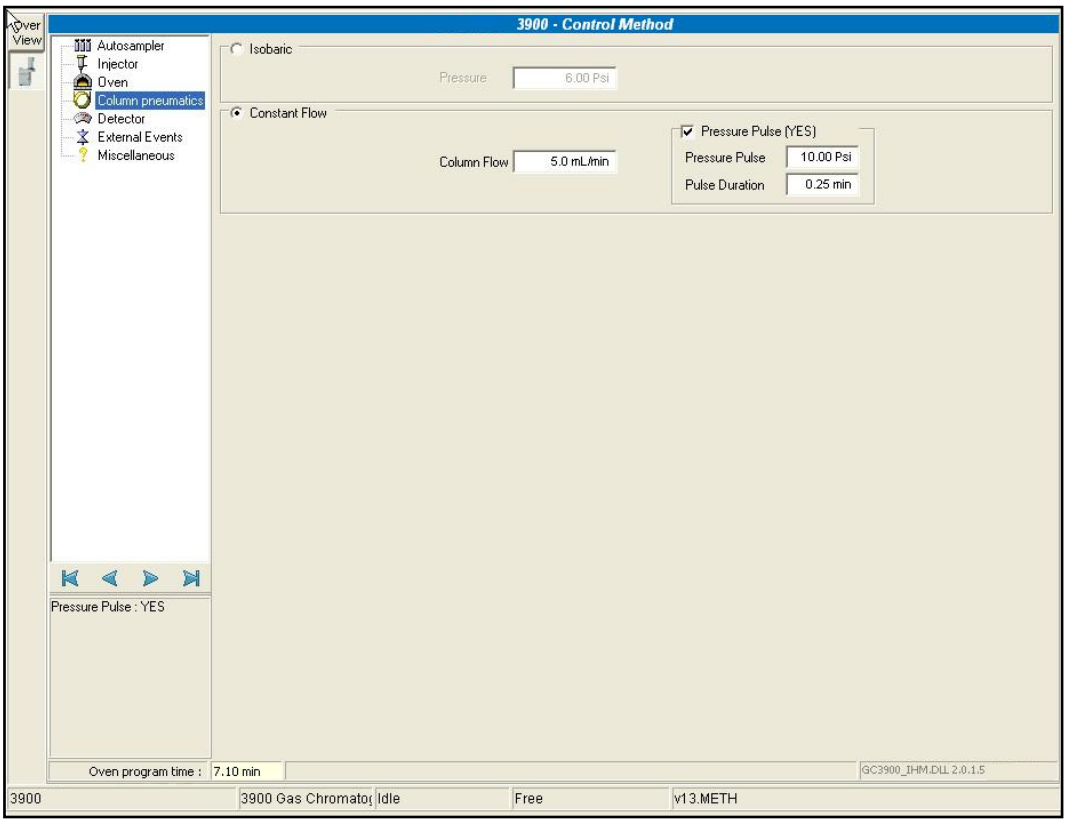
This parameter provides a safety measure to save coolant after the specified time if the column oven fails to reach its set temperature or the GC does not go into run. The valve will be turned OFF if the timeout period is reached and no further coolant will be applied.

NOTE: The browser always displays the current end time of the column oven program. If you enter program end times for components other than the column oven that exceed the column oven end time, a warning message will be displayed. The column oven end time determines the method end time. As a consequence, when the method is downloaded to the GC, component program end times that exceed the column oven end time will be truncated.

Column Pneumatics Control

The Column pneumatics window contains the Electronic Flow Control (EFC) Program which allows you to specify the pressure ramp of the Type 1 EFC or the pressure ramp and total flow time program of the Type 4 EFC. Type 1 EFC is specially used for the 1177 injector while Type 4 EFC is used for the 1041 injector.

Type 1 EFC



Isobaric Parameter Group

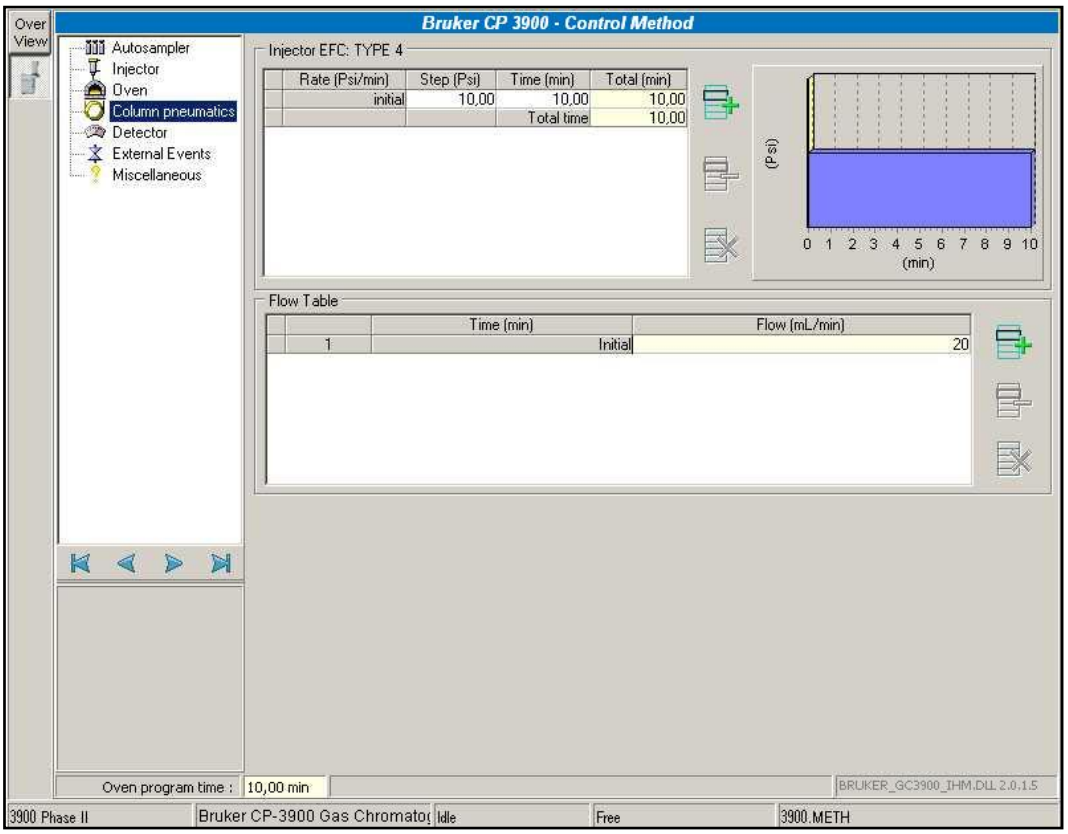
Check the Isobaric option to define a desired gas Pressure in the corresponding field.

Constant Flow Parameter Group

Check the Constant Flow option to disable the isobaric option and enter the desired constant Column Flow in the corresponding field.

Check the Pressure Pulse option to perform a pressure pulse injection. Prior to injection, the column head pressure will change to the Pressure Pulse pressure. After injection, the Pressure Pulse pressure will be maintained for the Pulse Duration.

Type 4 EFC



Injector EFC Parameter Group

Use the first spreadsheet to build a pressure ramp program.

The first row of the spreadsheet contains the Initial pressure and hold time for the Type 4 EFC. The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the programmed settings for each of the ramp segments. Enter the final pressure of each ramp segment in the Step column (0.10 to 400.00 Psi), the Rate (0.01 to 400.00 Psi/min) and the Time (0.00 to 999.99 min) the EFC is held at this pressure in the corresponding columns.

NOTE: The graph shows the pressure ramp program.

Flow Table Parameter Group

Use the second spreadsheet to build a flow time program to control the Type 4 EFC total flow.

The first row of the flow spreadsheet contains the Initial Total Flow for the Type 4 EFC.

The EFC will equilibrate to this setting when the method is activated, and will be restored to this setting when each chromatographic run is completed. The rest of the spreadsheet contains the time-programmed settings for the total flow. The total Flow (1 to 1000 mL/min) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min).

Use the following buttons to edit the table :

to add a line to the table.

to delete a line in the table.

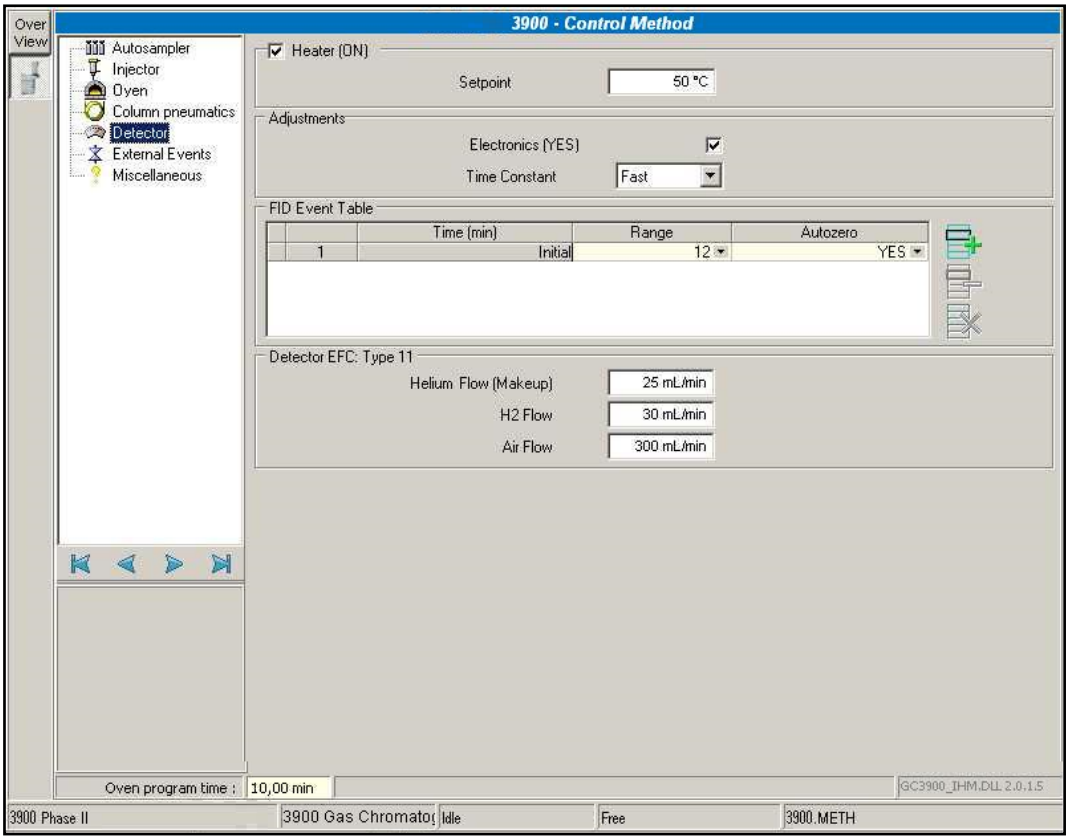
to clear the entire table.

.

Detector Control

The Detector sub-section allows you to specify the operating temperatures, gas flow rates, and specific parameters for the FID (Flame Ionization Detector) detector or the TCD (Thermal Conductivity Detector) detector.

FID Detector



Check or uncheck the Heater option to turn the detector oven ON or OFF and enter the detector oven temperature in the Setpoint field (50 to 450 °C).

Adjustments Parameter Group

Check or uncheck the Electronics option to indicate whether the installed FID will be used or not. Select the required Time Constant from the list (Fast or Slow).

FID Event Table Parameter Group

Use the spreadsheet to change detector settings during the analysis.

The first row of the spreadsheet contains the Initial Range and Autozero for the FID detector. When the autozero is set to yes, it means the detector autozero is on continuously before the run starts.

The rest of the spreadsheet contains the time-programmed settings: the Range (9, 10, 11, or 12) and Autozero (Yes or No) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min)

Use the following buttons to edit the FID event table:

to add a line to the table.

to delete a line in the table.

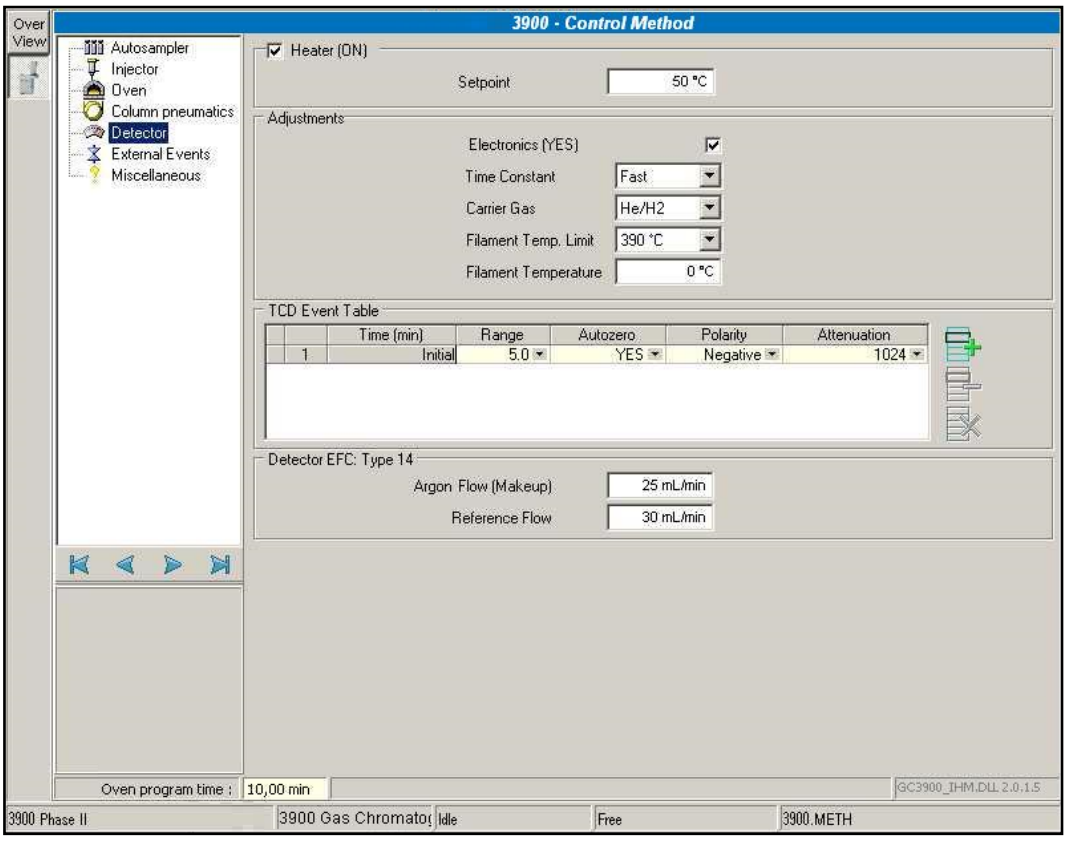
to clear the entire table.

Detector EFC Parameter Group:

The Type 11 EFC section allows you to define the desired gas flow rates [Helium Flow (Makeup), H2 Flow and Air Flow fields, 0 to 50 ml/min for the makeup and hydrogen flows, and 0 to 500 mL/min for the air flow].

NOTE: The Electronic Flow Control modules (EFC) are detector-specific and specified in the configuration manager. For FID detectors, the EFC Type 11 is required.

TCD Detector



Check or uncheck the Heater option to turn the detector oven ON or OFF and enter the detector oven temperature in the Setpoint field (50 to 450 °C).

Adjustments Parameter Group

Check or uncheck the Electronics option to indicate whether the installed TCD will be used or not. Select the required Time Constant from the list (Slow or Fast).

Choose the Carrier Gas: if you are using helium or hydrogen as carrier gas, select the He/H2 setting. For all other carrier gases, select the N2/Ar setting.

Specify the Filament Temperature in the corresponding field (0 °C to the maximum filament temperature) and select the Filament Temperature Limit from the list: to protect the filament, always operate the detector with the 390 °C limit selected unless you require the maximum dynamic range available to the TCD. With the limit set to 390 °C, the peak sample filament temperature is limited to approximately 450 °C. The temperature limit is approximately 550 °C at the 490 °C setting. The 450 °C limit protects filaments from oxidation when exposed to air over an extended period of time. However, at the 550 °C temperature limit the filament can degrade after only a few minutes.

TCD Event Table Parameter Group

Use the spreadsheet to change detector settings during the analysis.

The first row of the spreadsheet contains the Initial Range, Autozero and Polarity for the TCD detector. When the autozero is set to yes, it means the detector autozero is on continuous before

the run starts. The polarity is used to reverse the peaks that appear in the negative direction (for example, if you inject a standard or sample into the reference side of the TCD).

The rest of the spreadsheet contains the time-programmed settings: the Range (0.05, 0.5 or 5.0), Autozero (Yes or No) and Polarity (Positive or Negative) will be switched to the value in each row at the indicated Time (0.01 to 999.99 min).

NOTE: If you are also collecting the detector analog signal (via an analog output connected to a MIB-interface for example), you can define the required *Initial Attenuation* and change it during the analysis.

Use the following buttons to edit the TCD event table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

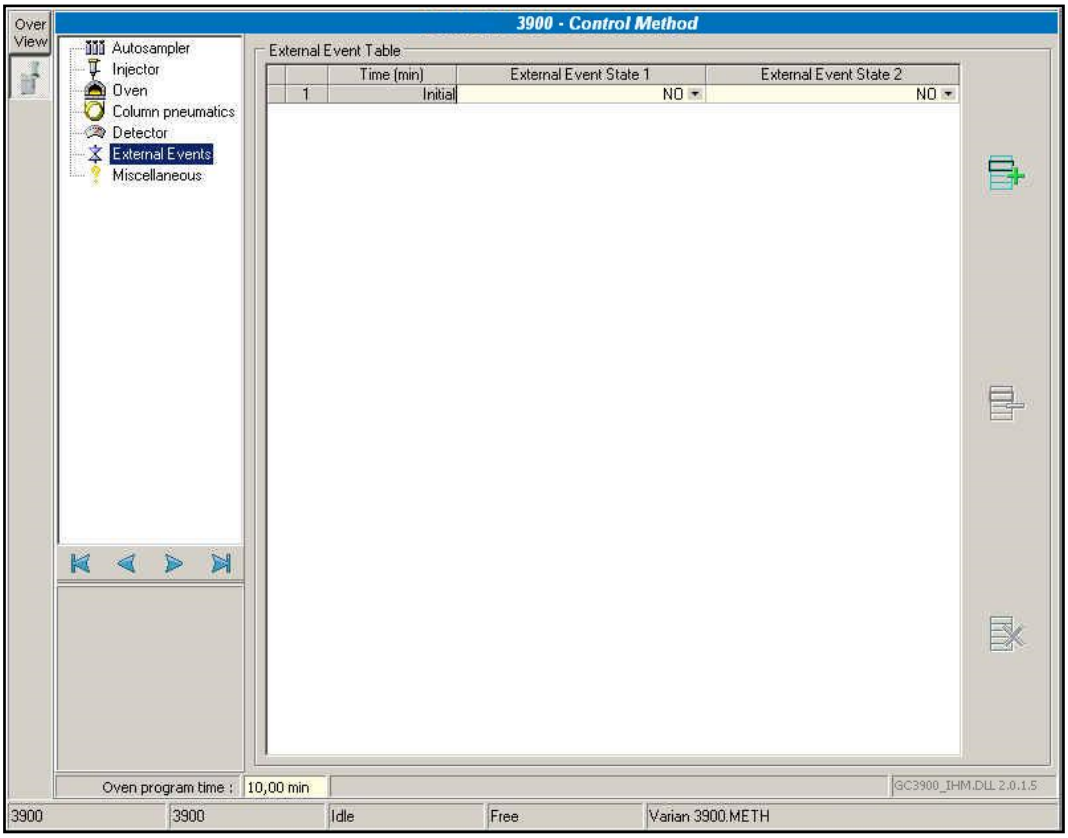
Detector EFC Parameter Group

If the detector Electronic Flow Control module is installed, the Type 14 EFC section will appear and allows you to define the desired gas flow rates (Makeup Flow and Reference Flow fields, 0 to 50 mL/min).

NOTE: The Electronic Flow Control modules (EFC) are detector-specific. For TCD detectors, The EFC Type 14 is required.

External Events Control

The 3900 GC can have up to two external events:



External Event Table Parameter Group

Use the spreadsheet to time program the external events. The first row of the spreadsheet contains the initial external events position. The External Event State 1 and External Event State 2 columns allow you to turn the relay associated with each external event ON (Yes) or OFF (No). :

Use the following buttons to edit the External Events table

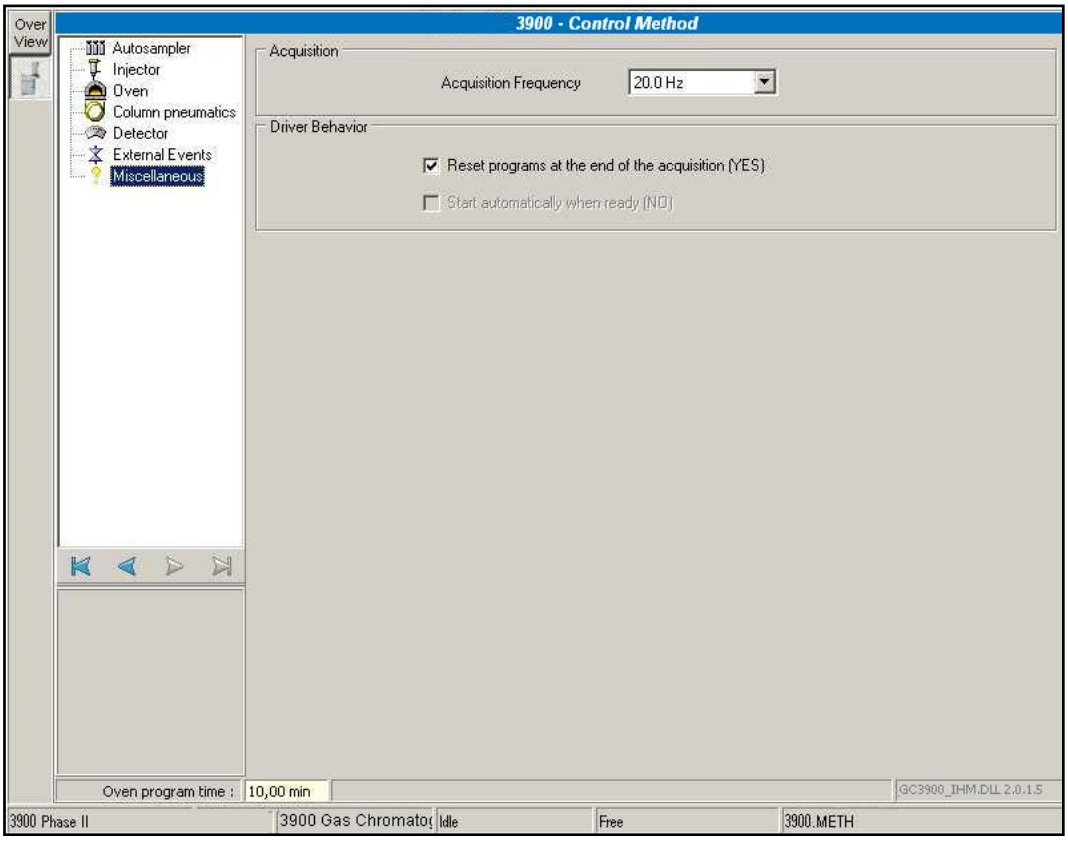
to add a line to the table.

to delete a line in the table.

to clear the entire table.

Miscellaneous Control

The Miscellaneous section contains parameters for data collection:



Acquisition Parameter

Enter the detector data rate in the Acquisition Frequency field. With decreased data rates, less disk space is required for storing the data. With increased rates, more data is collected, which may improve quantitation, particularly for narrow peaks.

Driver Behavior Parameter Group

Check or uncheck the Reset programs at the end of the acquisition to activate or deactivate this option. If it is checked and the acquisition is stopped from the acquisition window, the temperature programs will be reset before continuing with the next injection (if a sequence is running).

Check Start automatically when ready to start the GC without injecting. It could be useful in case of sampling valve use.

Starting and Viewing an Acquisition

Quick Start and Sequence

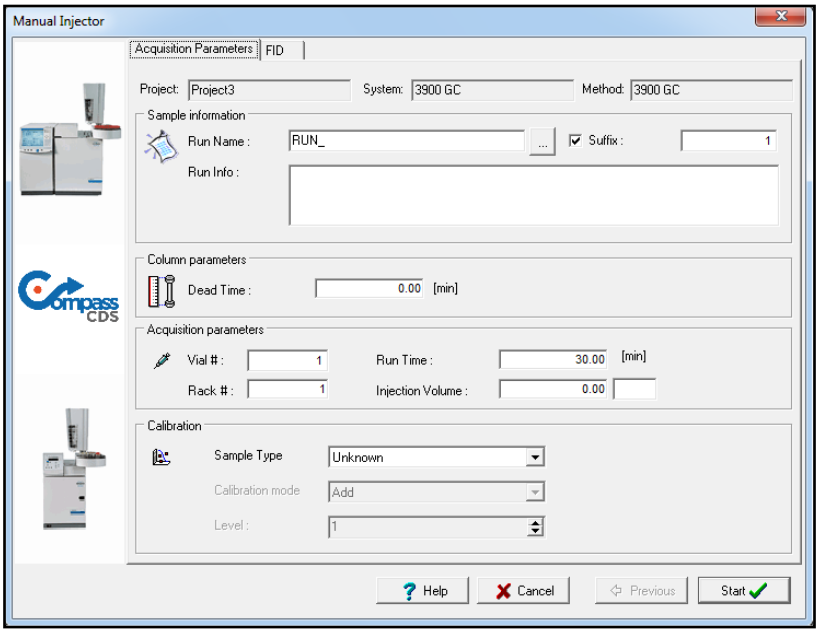
Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

Quick Start (Single Acquisition)

Press the button.

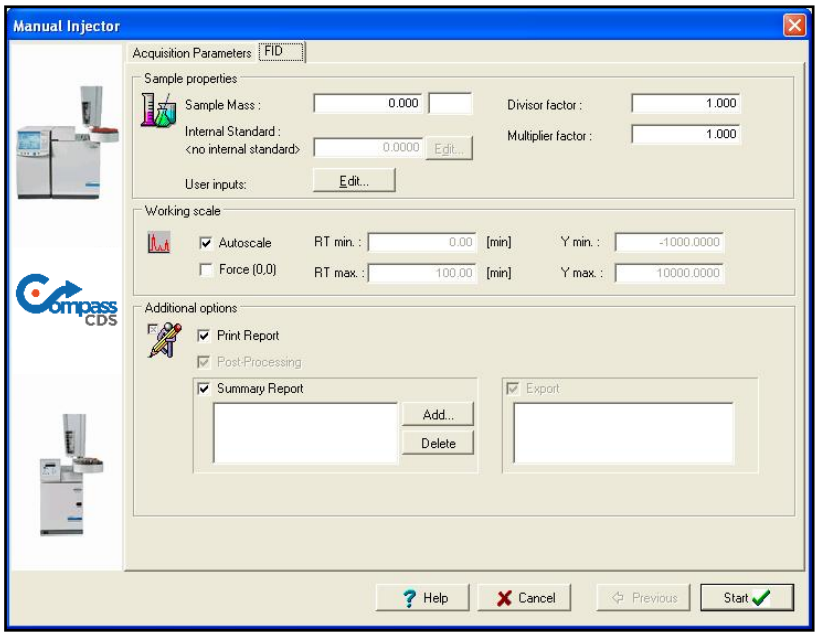
In the ***Quick Start*** window, select the system, the method, and optionally the project if connected in "All project" mode.

Press the OK button. The following screen is displayed:



In the *Acquisition parameters* tab, required fields like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by CompassCDS, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the *Channel X* or FID tab.

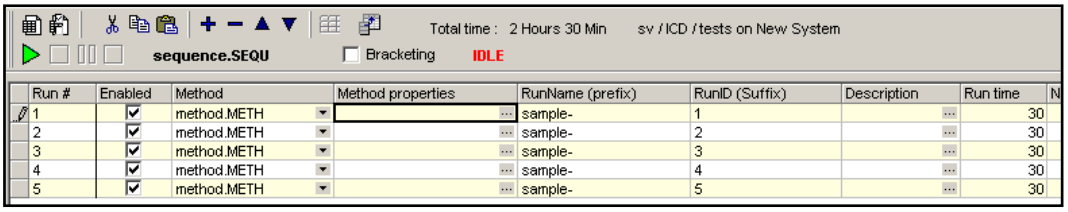


Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples) and the sequence name.

The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time	N
1	☑	method.METH		sample-	1		30	
2	☑	method.METH		sample-	2		30	
3	☑	method.METH		sample-	3		30	
4	☑	method.METH		sample-	4		30	
5	☑	method.METH		sample-	5		30	

The *Method Name*, the *Run Name*, the *Run ID* and the *Acquisition length* must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

To view a running acquisition, click on the Systems tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed. If Dual View is selected then the acquisition will be observed while the sequence is running.

Status of the 3900 GC

Click on the button corresponding to the 3900 GC driver and the 3900 status screen will appear. It contains eight sub-sections: Autosampler, Injector, Oven, Column, Detector, External Events, Miscellaneous, and Overview. Click on the required sub-section to display the corresponding parameters that will be used during the chromatographic run.

A toolbar allows you to easily scroll through the status windows:

to select the first status window.

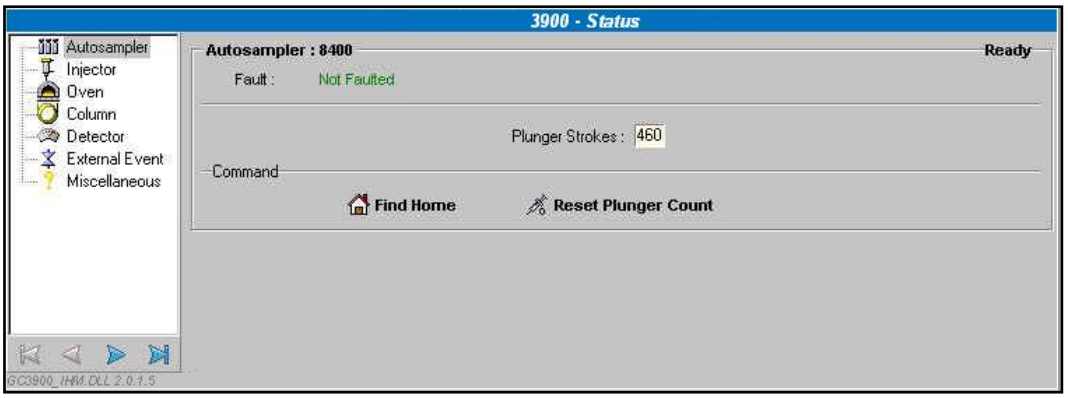
to move back to the previous status window.

to move forward to the next status window.

to select the final status window.

Autosampler Window

This section is only shown when 3900 GCs have either an 8400 Autosampler or an 8410 AutoInjector connected to them.



The autosampler status screen indicates the autosampler state (Ready, Homing, Sampling or Running).

Fault or No Fault: displays if a fault in the autosampler component has occurred. In this case, a new button appears:

. Click on it to clear the fault.

Plunger Strokes: displays the number of times that the syringe plunger has been moved up and down. This can be used to help monitor syringe wear and plan for syringe replacements.

Click on the

button to reset the number of plunger strokes.

Click on the

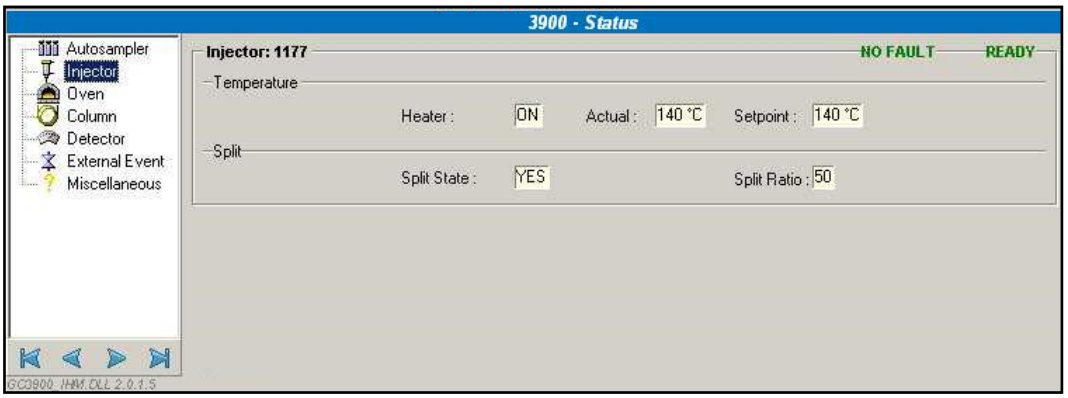
button to reinitialize the autosampler.

If an 8410 Autosampler is connected, the button

becomes available. Click on it to detect the tray orientation (1 to 10, 11 to 16 or 17 to 21).

Injector Window

1177 Injector



The following status parameters are available:

Ready or Not Ready: the injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”.

Fault or No Fault: displays if a fault in the injector component has occurred.

Heater: displays if the injector oven component is turned OFF or ON at the 3900 GC.

Actual: displays the actual temperature of the injector oven at the 3900 GC.

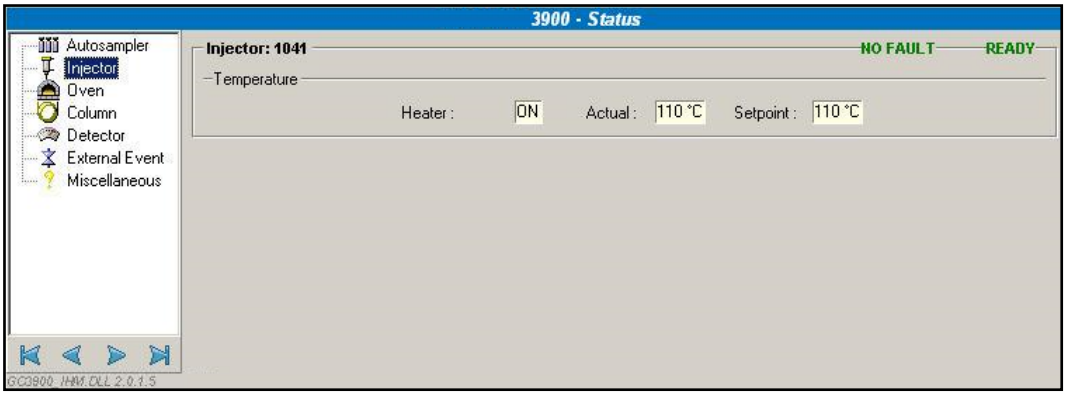
Setpoint: displays the injector oven programmed temperature setting in the active method. The 1177 injector is an isothermal injector.

Split State: displays the current split state of the 1177 injector method.

Split Ratio: displays the current split ratio of the 1177 injector method.

The split ratio is defined as the (Column Flow + Split Flow) / the Column Flow.

1041 Injector



The following status parameters are available:

Ready or Not Ready: the injector oven is Ready if the setpoints have been achieved and stabilized. The injector oven is Not Ready if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes “out of tolerance”.

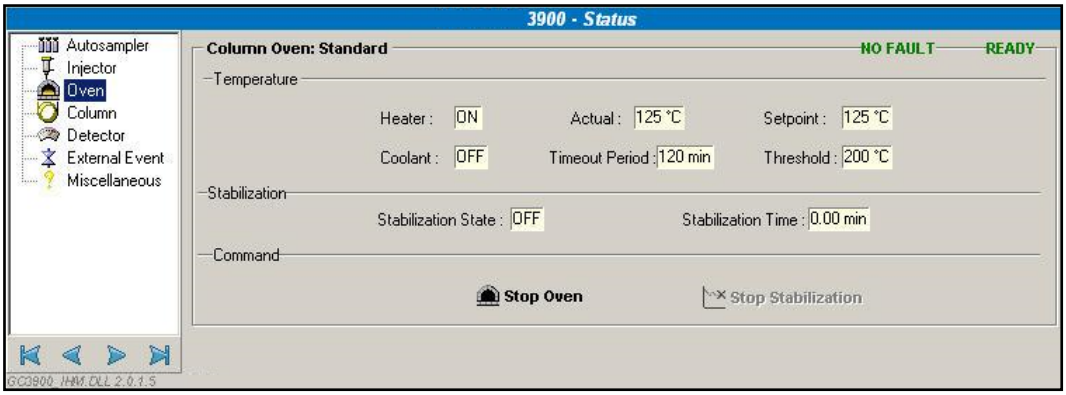
Fault or No Fault: displays if a fault in the injector component has occurred.

Heater: displays if the injector oven component is turned OFF or ON at the 3900 GC.

Actual: displays the actual temperature of the injector oven at the 3900 GC.

Setpoint: displays the injector oven programmed temperature setting in the active method.

Column Oven Window



The status display includes the following parameters:

Ready or Not Ready: the column oven is Ready if the setpoints have been achieved and stabilized. The column oven is Not Ready (No) if readiness to start a run has not been achieved or if, during a run, the oven becomes not ready or goes out of tolerance.

NOTE: Some reasons the GC may display Not Ready during a run are: the temperature program is too aggressive, the oven door is opened, the coolant runs out, or the power line voltage drops.

Fault or Not Faulted: displays if a fault in the column oven component has occurred.

Heater: displays if the column oven component is turned OFF or ON at the 3900 GC.

Actual: displays the actual temperature of the column oven at the 3900 GC.

Setpoint: displays the column oven programmed temperature setting in the active method.

Coolant: displays if the column oven coolant is enabled in the active method.

Timeout Period: displays the programmed coolant time-out value in the active method for the column oven.

Threshold: displays the programmed column oven temperature at which the column oven coolant is enabled.

Stabilization State: displays the current stabilization state of the oven. When the state is ON, the button

becomes active. Click on it to bypass the stabilization time.

Stabilization Time: shows the 3900 GC column oven stabilization time in minutes. The stabilization time counts down from the programmed method value and then displays 0.00 minutes when the stabilization period is over.

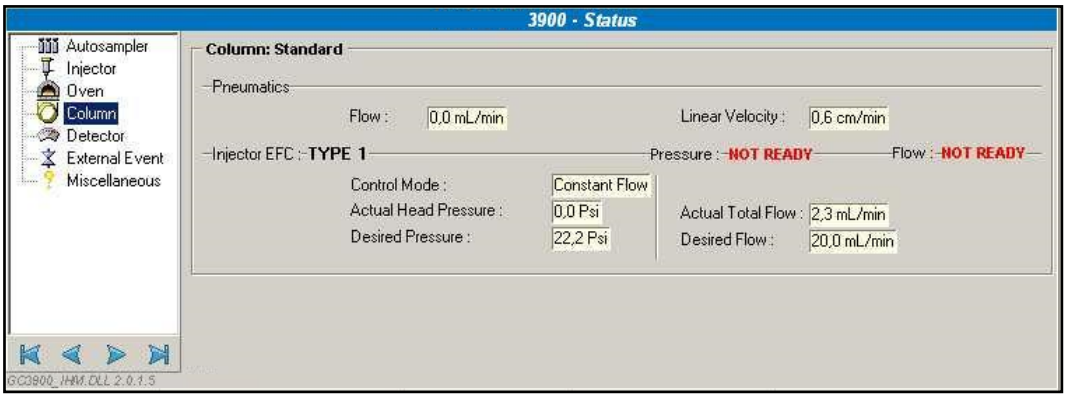
Click on

to turn off the oven when the oven is on.

Click on

to turn on the oven when the oven is off.

Column Window



The status display includes the following parameters:

Flow: displays, in mL/min, the column flow rate calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

Linear Velocity: displays the column linear velocity calculated from the column head pressure, column temperature, and column parameters (carrier gas, column length, and internal diameter).

The injector EFC type is mentioned (Type 1 for 1177 injector, Type 4 for 1041 injector)

Pressure: Ready or Not ready. The Injector EFC pressure is Ready if the setpoint has been achieved and stabilized.

Flow: Ready or Not ready. The Injector EFC flow is Ready if the setpoint has been achieved and stabilized.

Control Mode: displays the control mode of the EFC (isobaric, constant flow).

Actual Head Pressure: displays the actual column head pressure at the 3900 GC.

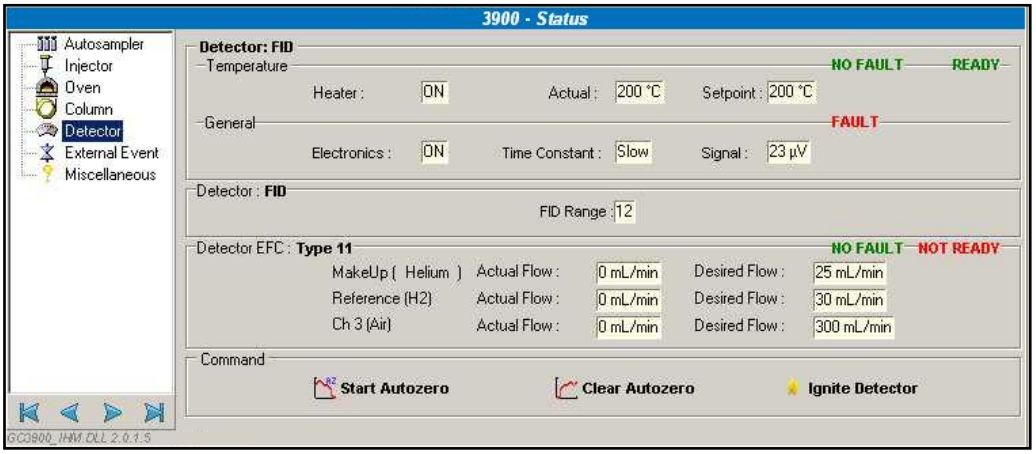
Desired Pressure: displays the programmed column head pressure setting in the active method.

Actual Total Flow: displays, in mL/min, the total flow rate through the system.

Desired Flow: displays the programmed column flow setting in the active method.

Detector Window

FID Detector



The status display includes the following parameters:
Temperature: Ready or Not Ready. The temperature of the FID detector is Ready if the setpoints have been achieved and stabilized.

Temperature: Fault or No Fault. Displays if a fault in the FID detector component has occurred.

Heated: displays if the detector oven component is turned OFF or ON at the 3900 GC.

Actual: displays the actual temperature of the detector oven at the 3900 GC.

Setpoint: displays the detector oven programmed temperature setting in the active method.

Electronics: displays the FID Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: displays, in mV, the actual FID detector signal at the 3900 GC.

FID Range: 9, 10, 11, or 12. Displays the FID Range initial condition setting or the time-programmed setting in the active method.

If the detector Electronic Flow Control module is installed, the Type 11 EFC section will appear and displays the following parameters:

Detector EFC: Ready or Not Ready. The Detector EFC is Ready if the setpoints have been achieved and stabilized.

Fault or No Fault: displays if a fault in the Detector EFC component has occurred.

Make Up: displays, in mL/min, the setpoint and actual channel 1 flow rate (Make up).

Reference: displays, in mL/min, the setpoint and actual channel 2 flow rate (Hydrogen).

Ch 3: displays, in mL/min, the setpoint and actual channel 3 flow rate (Air).

Click on the

button to ignite the detector flame.

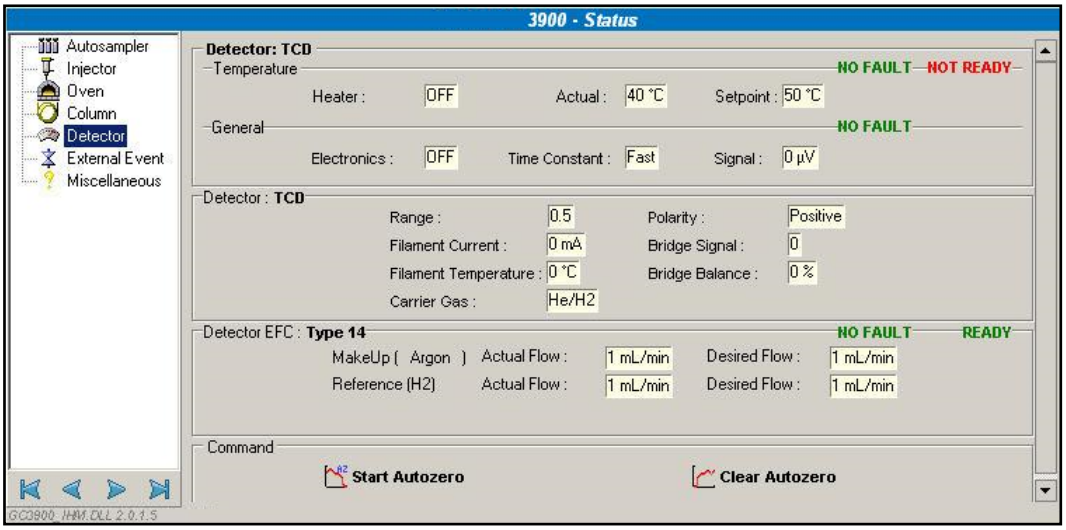
Click on the

button to launch the autozero of the detector.

Click on the

button to clear the autozero of the detector and get the raw signal from the detector (useful in case of diagnosis situation).

TCD Detector



Heater: displays if the detector oven component is turned OFF or ON at the 3900 GC.

Actual: displays the actual temperature of the detector oven at the 3900 GC.

Setpoint: displays the detector oven programmed temperature setting in the active method.

Ready or not ready: the TCD detector is Ready if the setpoints have been achieved and stabilized. The TCD detector is Not Ready if readiness to start a run has not been achieved or if, during a run, the TCD detector becomes not ready or goes “out of tolerance”.

Fault or No Fault: displays if a fault in the TCD detector component has occurred.

Electronics: displays the TCD Electronics setting in the active method.

Time Constant: Fast (50 msec) or Slow (200 msec). Displays the electrometer time constant setting in the active method.

Signal: displays, in µV, the actual TCD detector signal at the 3900 GC.

Range: 0.05, 0.5, or 5.0. Displays the TCD Range initial condition setting or the time-programmed setting in the active method.

Filament Current: displays, in mA, the actual TCD current.

Filament Temperature: displays the TCD Filament Temperature setting in the active method.

Carrier Gas: displays the carrier gas setting in the active method.

Polarity: displays the TCD polarity initial condition setting or time-programmed setting in the active method.

Bridge Signal: displays the actual TCD bridge signal.

Bridge Balance: displays the TCD bridge balance (%).

The Type 14 EFC section will display the following parameters:

Ready or Not Ready. the detector EFC is Ready if the setpoints have been achieved and stabilized.

Fault or No Fault: displays if a fault in the detector EFC component has occurred.

Make Up: displays, in mL/min, the setpoint and actual channel 1 flow rate.

Reference: displays, in mL/min, the setpoint and actual channel 2 flow rate.

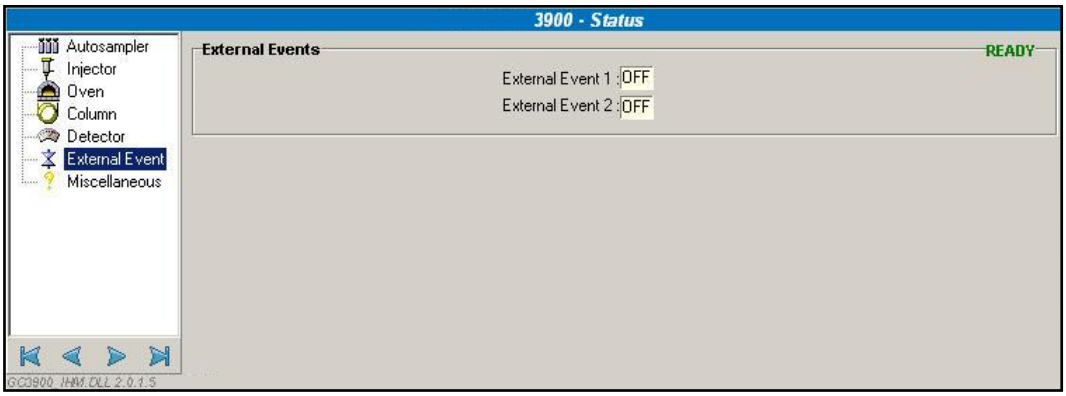
Click on the

button to launch the autozero of the detector.

Click on the

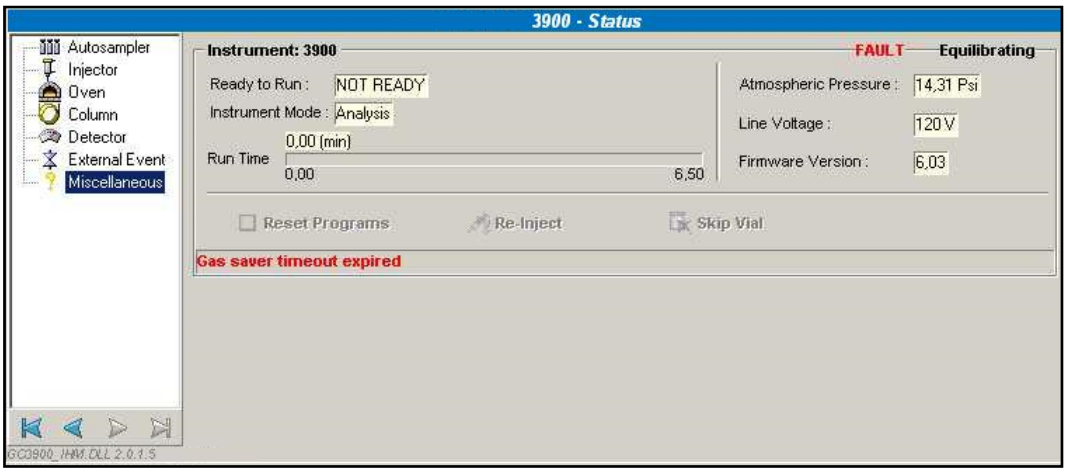
button to clear the autozero of the detector and get the raw signal from the detector (useful in case of diagnosis situation).

External Events Window



The status screen displays the current state of each external event.

Miscellaneous Window



The miscellaneous screen contains general information about the current run, the overall state of the instrument and the GC Firmware Version.

The state of the instrument (Ready, Running, Stabilizing, Equilibrating, Computing, Needs Monitor, Monitoring, Sampling, Connecting, or Not Ready) is displayed.

A Fault / No Fault indicator is also shown. When a hazardous or disabling fault occurs, any run in progress will halt and the affected component will shut down. If the fault is recoverable, then the run is not terminated.

The run time bar displays the elapsed time in minutes since the beginning of the run and the end time.

Atmospheric Pressure: displays the current value of the atmospheric pressure calculated by the GC.

Press the

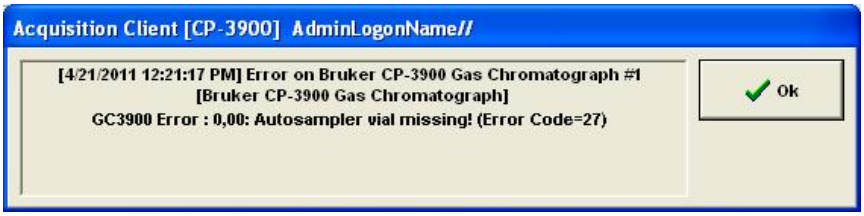
button, to reset the GC. If it is RUNNING, the GC aborts the current run, goes to the READY state and continues with the next injection in the sequence. This button is equivalent to pressing the Stop on the front panel of the GC.

When a vial is missing during a sequence, a warning message appears and you have 10 minutes to replace the sample in the correct position before the system skips the missing vial and passes to the next line of the sequence, or stops the run. When you have replaced the missing sample, you must press the

button to restart the run.

If you want to skip the missing vial and start the next run, you must press the

button.

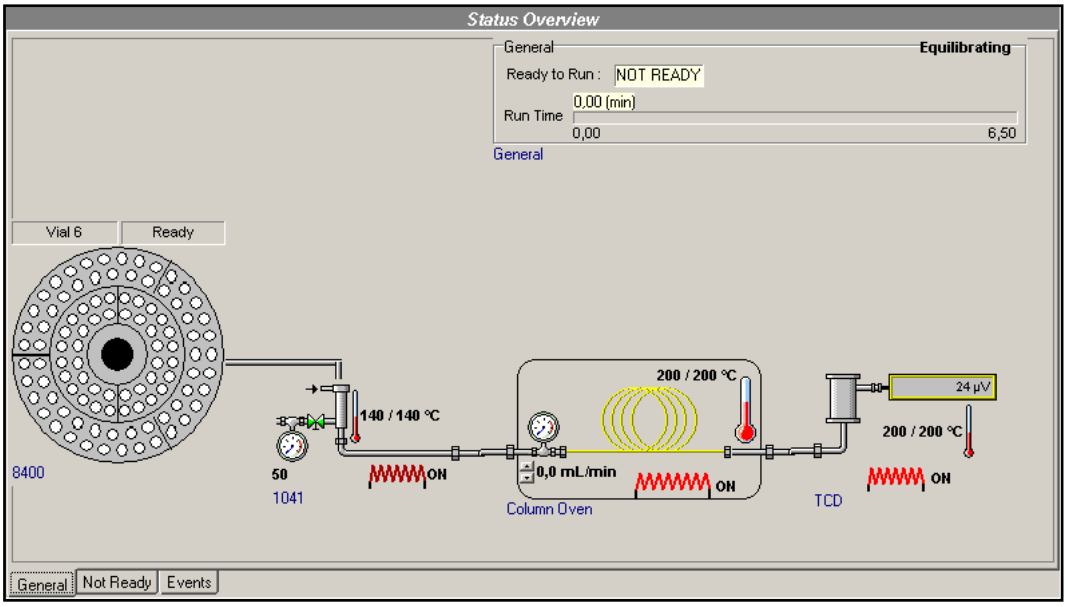

Acquisition Client [CP-3900] AdminLogonName//
[4/21/2011 12:21:17 PM] Error on Bruker CP-3900 Gas Chromatograph #1
[Bruker CP-3900 Gas Chromatograph]
GC3900 Error : 0,00: Autosampler vial missing! (Error Code=27)
Ok

Warning message when a vial is missing.

Overview Window

Click on the Over View button: the Status Overview window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (temperatures, pressures, and signal).



When the mouse points to a colored vial (yellow for current vial, green for already used vial and red for missing vial), the current vial number and the number of injections are displayed.

The flow and temperature (current and setpoint) for each module and the signal values are displayed. You can choose to display the flow, the pressure or the velocity of the gas in the column by clicking on the button.

Not Ready: contains the not ready information sent by the instrument.

Events: contains the events that have occurred on the instrument, listed below:

3900 GC Faults

-5V / +5V out of range	The –5V / +5V power lines are outside of their allowed tolerance for correct GC operation.
ADC Calibration failure	Activate a method to clear this fault. If the fault recurs, turn the GC off and then on.
Board Failure	The 3900 just detected that the specified detector has a failed electronics board.
DAC Calibration failure	The DAC (Digital to Analog Converter) that supplies the analog output signal failed to calibrate within its set tolerance. Turn off the power and then turn it back on.
DIAG Temp. out of range	The actual temperature of a temperature controlled resistor block used for automatic instrument calibration has exceeded its allowed temperature set point. Turn the power to the GC off and then on again.
Fan unplugged during run	Turn off instrument and turn it back on.
FID Flame out	The FID flame has been quenched. The flame detection is based on a background signal intensity of approximately 330 microvolts. It is possible for very clean GC systems to have baselines less than 330 microvolts causing spurious flameout messages. If you suspect that the flameout message is spurious, use a shiny, cool metal object (such as a box end wrench) and hold it just above the FID tower being careful not to get too close to the hot surfaces. If you observe condensation, then the flame is still lit; you may wish to change your fuel gas mixture or some other operating characteristic that would allow a slightly higher background signal. Once a flame out is detected, the system will attempt to ignite the flame 3 times before reporting the flame out condition. The fault is cleared by either igniting the flame using the Ignite FID Flame! Command or by turning the Detector electronics off and then on again.
Gas saver timeout expired	The GC has been idle for a period of time equal to or greater than the set Gas Saver timeout period. Activate a method to clear the fault.
Internal Temp. limit exceed	Turn off instrument and turn it back on.
IOP Communication failure	Turn off instrument and turn it back on.
Lower than minimum temp	The 3900 just detected that the specified component temperature zone has gone below its minimum temp.
Max setup temperature limit exceeded	The 3900 just detected that the specified limit exceeded component temperature zone has exceeded its maximum setup temperature limit.
Maximum temp has been exceeded	The 3900 just detected that the specified component temperature zone has exceeded its maximum temperature.
Step motor moving	The column oven vent stepper motor has failed to reach its internally set position within the step tolerance. Turn the power off and then on again
Temp probe is open	The 3900 just detected that the specified component temperature zone probe has an open circuit.
Temp probe is shorted	The 3900 just detected that the specified component temperature zone probe has a short circuit.
Temp probe response is too fast	The 3900 just detected that the specified component temperature zone probe is responding too fast.
Temp probe response is too slow	The 3900 just detected that the specified component temperature zone probe is responding too slowly.
Thermal runaway	The 3900 just detected that the specified component temperature zone has begun thermal runaway.

Autosampler Faults

84x0 communication	The Autosampler/AutoInjector has experienced an error during communications that was unrecoverable. Power off both your GC and the autosampler, Turn on power to the GC followed by turning on the power to the autosampler.
84x0 faulted	The A/S has failed to properly come up. Turn off the power and then turn it back on.
84x0 carousel error	The A/S carousel base has encountered one or more internal faults and has failed to properly come up. Turn off the power and then turn it back on.
84x0 carousel sensor not found	The autosampler carousel sensor has failed to conform to its expected operation. Turn the GC off then on again.
84x0 maximum plunger speed exceeded	This message is displayed if you have built a method with one syringe that supports a fast injection speed and have subsequently changed and configured a different syringe. Correct the syringe speed in your method for the new syringe
84x0 plunger error	The syringe plunger has either jammed or become inoperable. Check that the syringe is properly mounted and that you have free movement of the plunger. Replace the syringe if required.
84x0 plunger strokes exceeded limit	This is an advisory message that the plunger limit stroke count has exceeded the limit that was set for it. You should change the syringe and zero the plunger stroke counter soon after you observe this message.
84x0 plunger sensor not found	The autosampler plunger sensor has failed to conform to its expected operation. Turn off the GC and then on again.
84x0 run not started after injection	Restart Automation to clear this fault. If it recurs, check that the inject switch installed on the injector nut is functioning properly.
Run ended before injection	The autosampler failed to complete the injection sequence. Restart a run to clear the fault
84x0 syringe sled sensor not found	The syringe sled is either jammed or miscalibrated. Recalibrate your vial and injector positions making sure that the syringe sled has a small clearance (consult your manual) above vials and does not compress the injector switch on the injector.
84x0 syringe volume exceeded	The total volume of the sample, air gaps (if any), solvent plugs (if any), and internal standards (if any) exceeds the capacity of the configured syringe. Note that this error is only sensed at the time of injection. Check your method and correct any volumes that are excessive.
84x0 syringe missing	The autosampler has sensed that the syringe is not installed. Check that you have a syringe installed.
84x0 tower error	The autosampler tower has one or more internal faults and has failed to properly come up. Turn off the power and then turn it back on.
84x0 tower sensor not found	The tower sensor does not conform to its expected operation. Turn the GC off and then on again.
84x0 tray is missing	The 8410 sample tray has been removed from the base. Replace the tray; the 8410 should automatically sense that the tray has been replaced.
84x0 vial missing	The autosampler has failed to detect a vial within an expected range of vials. This message is an advisory message. If you have a vial in the position and it has been missed, check that a septum is installed. Lack of a septum and dark colors may cause the tower sensor to fail to identify the vial.
84x0 vial sensor bad	The autosampler vial sensor has failed to conform to its expected operation. Turn off the GC and then on again.
8410 Vial is unreachable	This message informs you that the 8410 tray is oriented such that the requested sample vial does not fall under the arc of the tower. Re-orient the tray or change the requested vial from which you intend to inject to correct this

Varian SHS-40 Headspace Autosampler Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501550
Revision B

Contents

Introduction....3
Installation and Configuration....3
Building a Method....5
Setting the Run-Time....6
Remarks about SHS-40 methods and CompassCDS methods....7
Using the Acquisition – Rack parameter and vial number....7
Building a Sequence Method....7
Working with CompassCDS Version 4.0....7
Starting and viewing an acquisition....9
Handling Missing Vials....11

Introduction

This document describes the installation and configuration of the Varian SHS-40 Headspace Autosampler Control Driver for CompassCDS.

It also explains how to build a control method or a sequence for this SHS-40, how to start and view a running acquisition.

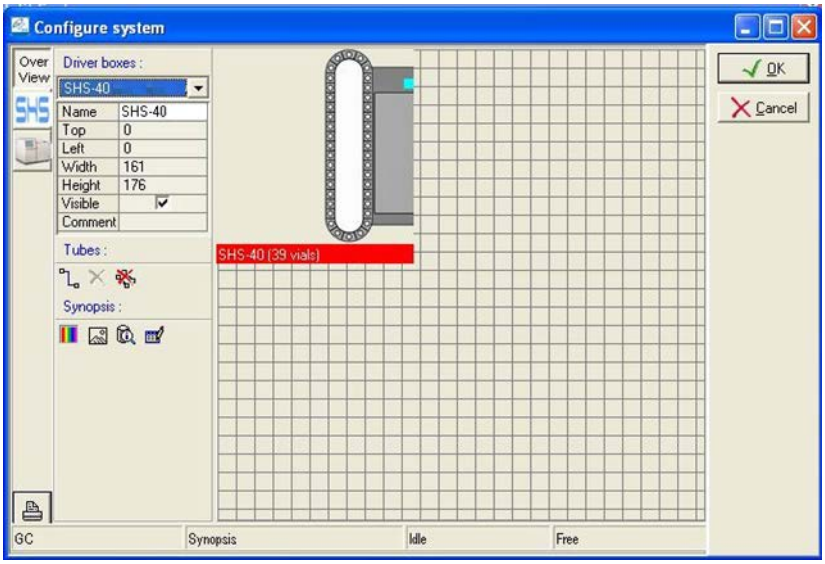
Installation and Configuration

The installation of the SHS-40 must be fully completed (see Installation Manual BR501547) with focus on the chapter “connecting to the data-system”.

The CompassCDS software must be installed (refer to the CompassCDS User Guide) before installing the SHS-40 driver software.

- Install the SHS-40 Driver software using the link (Install SHS-40 CompassCDS Driver).
- The SHS-40 drivers are now added to CompassCDS and can be used in the CompassCDS system.

To configure the SHS-40 in the CompassCDS Configuration Manager, click the right mouse-button on the desired system and choose ‘edit’.



There is one setting to configure the SHS-40:

- Choose the COM-Port to which the device is connected.

Figure 1 Configure the SHS-40

Building a Method

The following parameters must be entered in a method for the SHS-40:

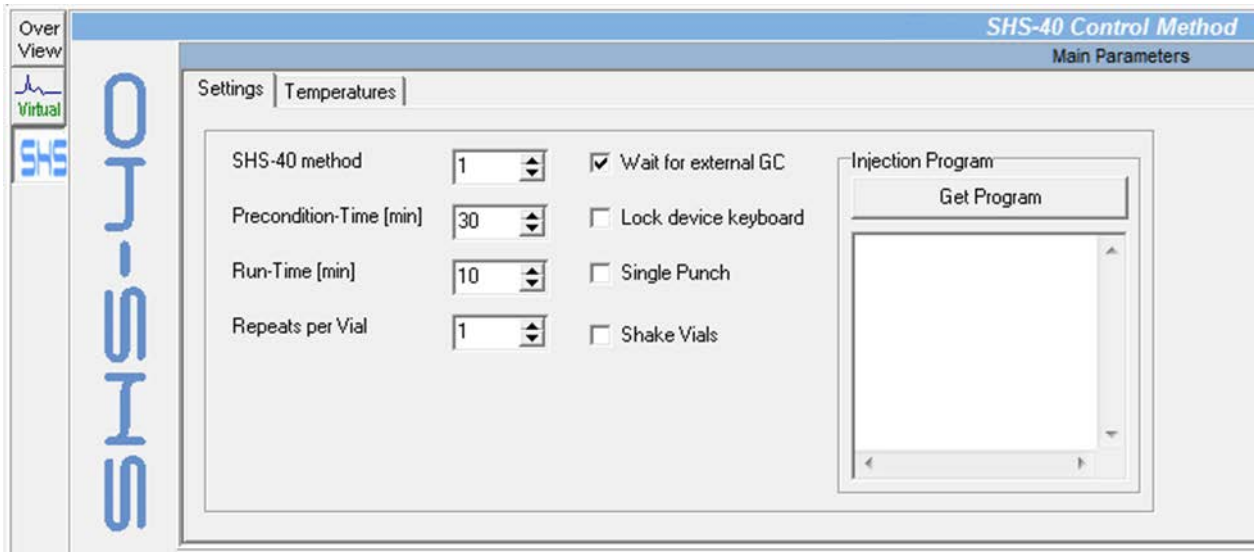


Figure 2 Method Parameters Settings tab

Parameters of the Settings tab:

Parameter	Range	Default	Description
SHS-40 method	1..9	1	Method to execute on the SHS-40. These methods can differ in the injection programs they execute.
Precondition-Time	1..300 min	30	Time to precondition the vial in the oven.
Run-Time	1..99 min	10	Run-Time of the analysis, see later remarks for setting the Run-Time.
Repeats per vial	1..9	1	Number of injections per vial.
Wait for extern GC	Yes/No	Yes	Wait for ready-signal of GC before injecting. Should always be enabled.
Lock device keyboard	Yes/No	No	Prohibit use of device keyboard during acquisition.
Single punch	Yes/No	No	If single punch is enabled, needle will penetrate the sample only once.
Shake vials	Yes/No	No	Shake vials

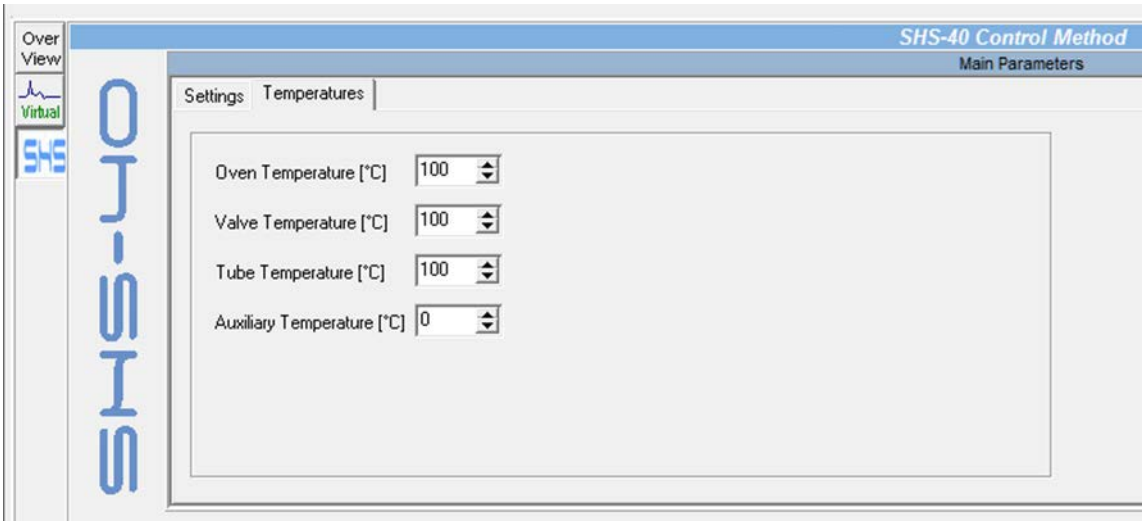


Figure 3 Method Parameters Temperatures tab

Parameters of the Temperatures tab:

Parameter	Range	Default
Oven temperature	0..200 °C	100
Valve temperature	0..200 °C	100
Tube temperature	40..200 °C	100
Auxiliary temperature	0..200 °C	0

Setting the Run-Time

Check the Run-Time entered in the GC, before setting the SHS-40 Run-Time parameter.

To let the SHS-40 work correctly you have to calculate the Run-Time for the SHS-40 as follows:

- Run time SHS-40 = 2 x GC Stabilization Time + GC-Oven program Time + 1 min System Ready Time + Oven cool down time

Before and after the GC data-acquisition, the GC stabilizes its temperatures for the entered stabilization time.

The System Ready Time is needed for safety reasons. This additional time ensures that the GC is waiting for injection (ready) when the SHS-40 starts the injection. Unfortunately it is possible that the GC sends a Ready-Signal when CompassCDS is in the Idle state. When the SHS-40 is waiting for injection, it will start injection, although CompassCDS is not in the Waiting-For-Injection phase.

The acquisition time entered in the method or a sequence for all devices is neglected when the system includes a Scion Instruments GC.

The described behavior may be different with gas chromatographs other than the Scion Instruments GC.

Remarks about SHS-40 methods and CompassCDS methods

In general, a CompassCDS method analyzes one sample at a time.

If more than one sample will be analyzed, this needs to be done with a sequence in CompassCDS.

To execute a SHS-40 method, you need to generate a CompassCDS sequence with one sample for every sample in the SHS-40 method. You will get one chromatogram for each analyzed sample.

The SHS-40 is started once and works without further instructions.

Using the Acquisition – Rack parameter and vial number

As already mentioned, the SHS-40 gets the instructions once and then works without further commands. These instructions have to be sent in the first sample of a sequence.

NOTE: The rack parameter of the acquisition settings or the rack parameter of the sequence needs to be modified in order to correctly instruct SHS-40 on how many samples (runs) are planned for a method. Therefore, set the acquisition rack parameter to '5' when analyzing five samples.

Set the rack parameter of the first sample in the sequence to the sample number and for all other samples of the same method to ‘0’ If you have a sequence consisting of samples from different methods, you need to set the rack parameter to the number of samples for the same method for every first sample of each method.

Building a Sequence Method

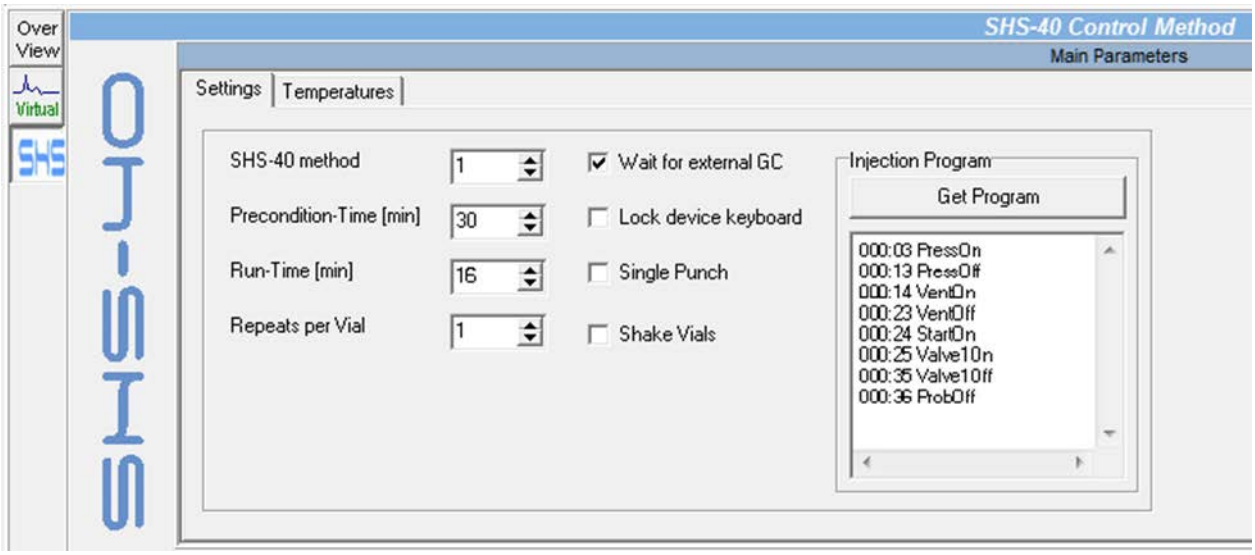
Working with CompassCDS Version 4.0

- Open a sequence and enter the desired Method (here STD_4a.METH)
- Description: Fill in the sample name.
- Vial: Fill in the corresponding SHS-40 vial position at the SHS-40 tray.
- Enter 5 at Rack# to analyze 5 samples at the first series.
- Fill in all five lines with correct data.

It is possible to program direct a second series, for example, with a different Method or with additional samples.

In the above example we add 3 samples and start with Position 6. All SHS-40 parameters are present in the method:

In the Control Method under “Control” and “SHS-40” are two tabs: Settings and Temperatures.

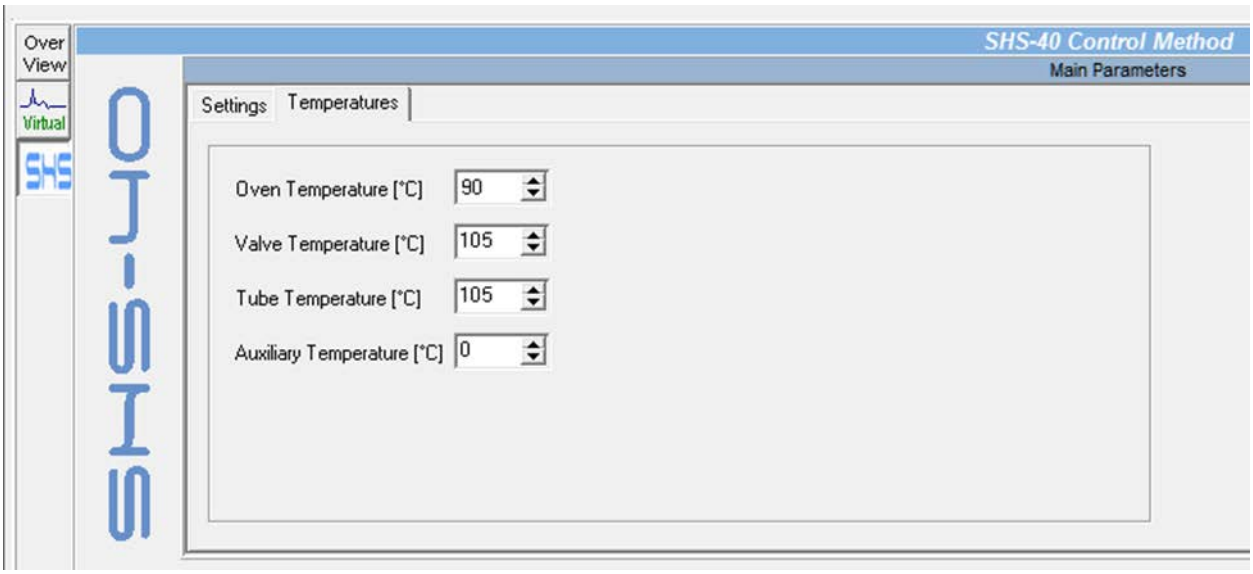


Please note that the “Run-Time” for the SHS-40 is the time which the GC needs for the GC run AND for cooling down (including equilibration time).

The “Precondition- Time” is the time which the SHS vial is headed up before the injection program started. The Precondition-Time is automatically calculated when a sample is placed in the oven (maximum 12 samples).

It is possible that there could be vials in the oven before the first GC run has been started (e.g., PC time 60 minutes; GC time 20 minutes).

Usually the temperatures of the valve and the tube must be higher than those set for the oven (remember the safety information for the oven temperature).



The oven temperature must be below 90 °C when water is present in the sample. Water in the vial will decrease the sensitivity of other components.

If the parameter Repeat per vial is greater than one, you have to multiply the samples in the sequence by the value of Repeats. If in the example the parameter Repeats was 2 for the first method, you should have entered 10 samples for this method.

The parameters Run time, No. of Injections, and Injection Volume of a CompassCDS sequence are not used by the SHS-40.

Starting and viewing an acquisition

In the SHS-40 status display, Method Settings tab, (see Figure 4) the parameters of the currently executed method are visible.

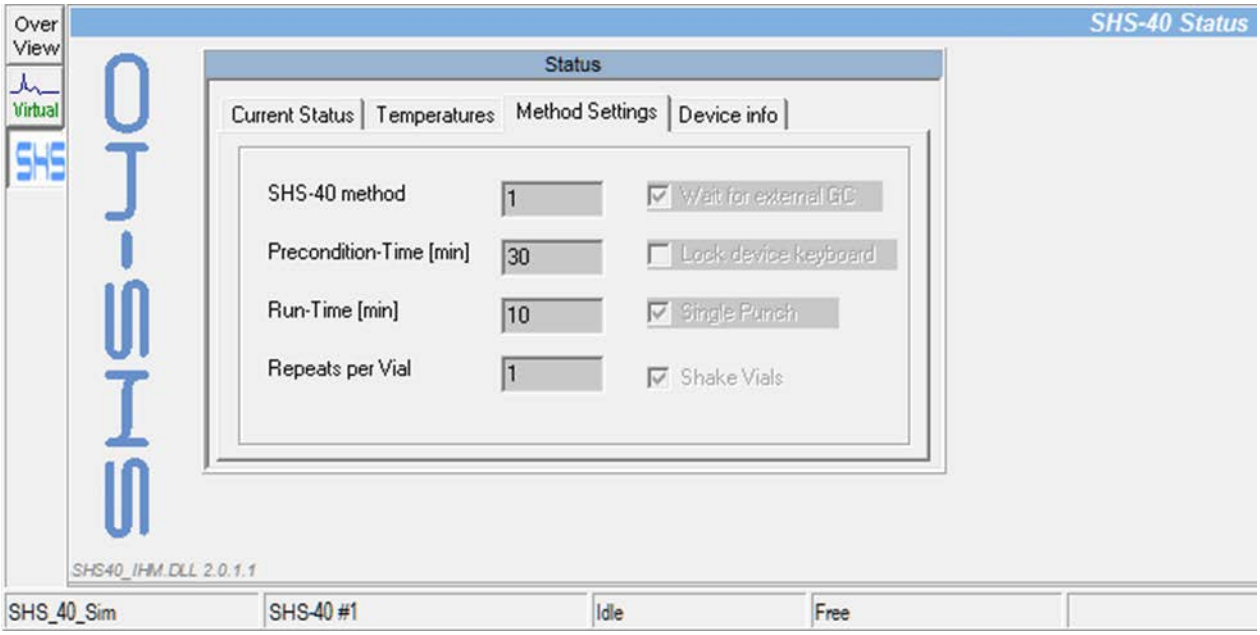


Figure 4 Status display of the SHS-40 during acquisition, Method Settings tab

The (Actual value) temperatures in the Temperatures tab are updated every 10 seconds from the SHS-40 (see Figure 5).

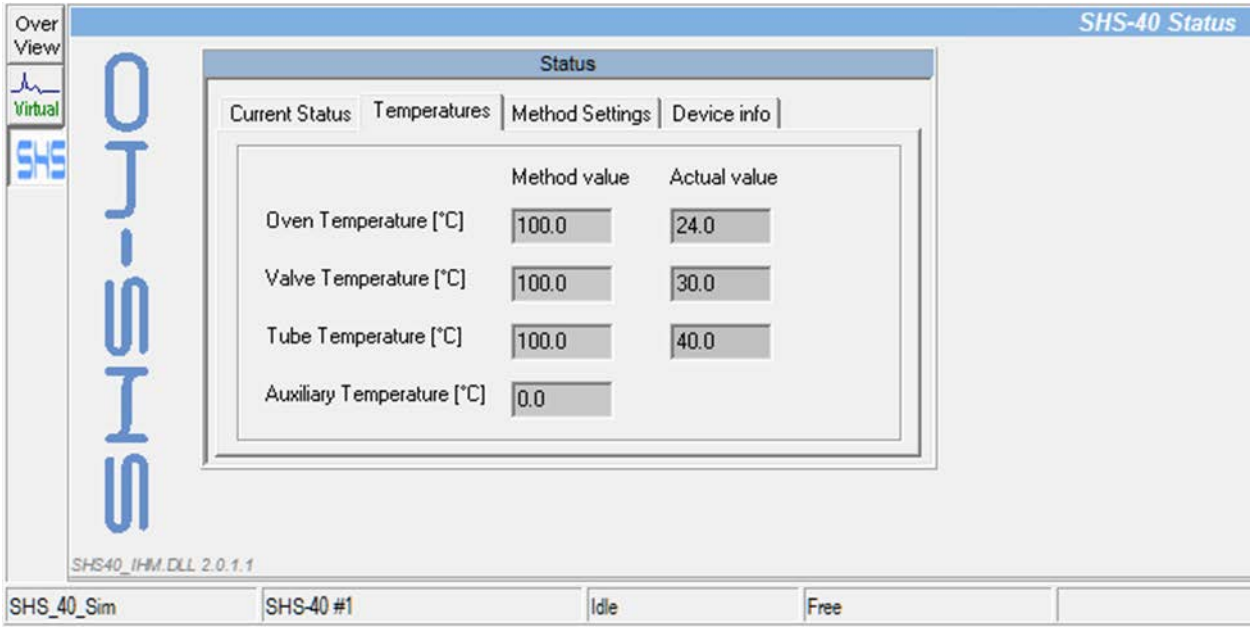


Figure 5 Status display of the SHS-40 during acquisition, Temperatures tab

The Current Status tab (Figure 6) shows two status lines (updated every 10 seconds) and the current stop vial.

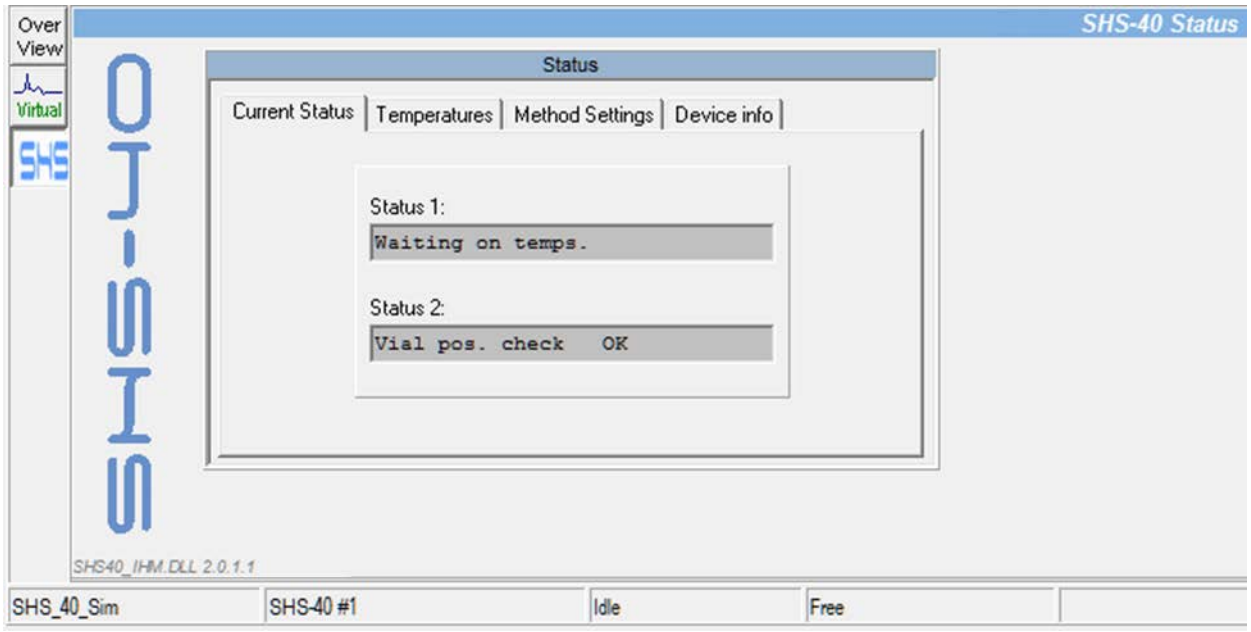


Figure 6 Status display of the SHS-40 during acquisition, Current Status tab

The Device info tab shows information about the attached device (see Figure 7).

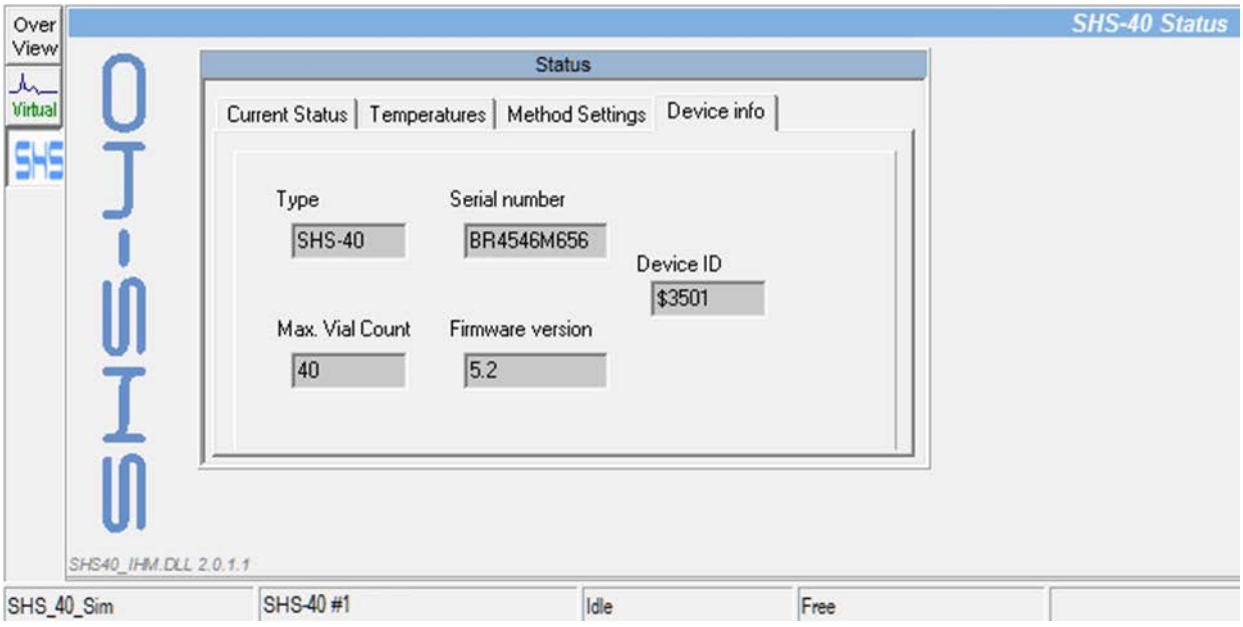


Figure 7 Status display of the SHS-40 during acquisition, Device info tab

Handling Missing Vials

The SHS-40 can recognize missing vials when trying to inject them.

Although a vial is missing, the SHS-40 sends an injection signal so that the CompassCDS sequence is not missing a sample.

The result of a missing vial is an empty chromatogram in the sequence. All other samples should have been analyzed correctly.

If a vial is missing or a vial was damaged during injection, the corresponding error message is written to the Run Log, which is part of a chromatogram-file.

Open the chromatogram, click the method section and view the acquisition parameters. On this dialog press the Run Log button and the Run Log will be displayed (see Figure 8).

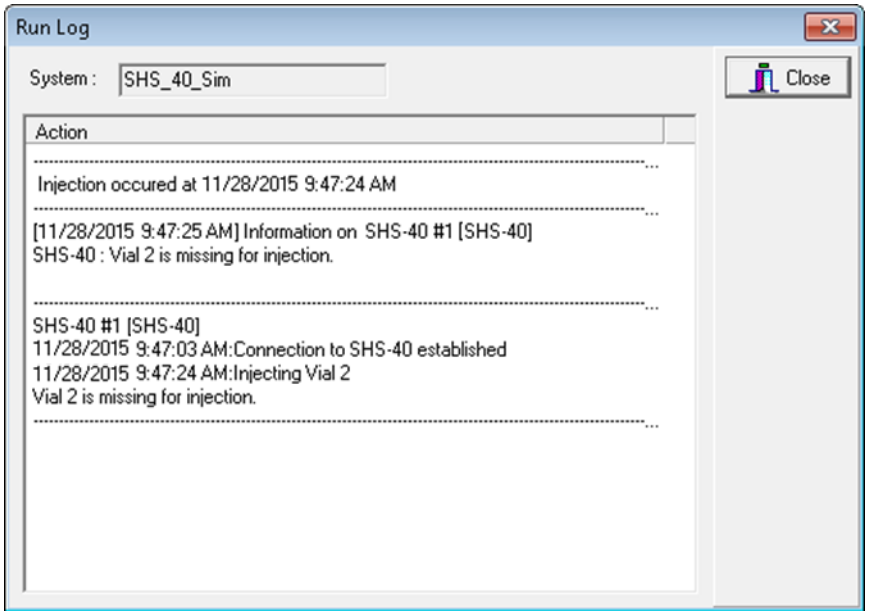

Run Log
System :
SHS_40_Sim
Close
Action
Injection occured at 11/28/2015 9:47:24 AM
[11/28/2015 9:47:25 AM] Information on SHS-40 #1 [SHS-40]
SHS-40 : Vial 2 is missing for injection.
SHS-40 #1 [SHS-40]
11/28/2015 9:47:03 AM:Connection to SHS-40 established
11/28/2015 9:47:24 AM:Injecting Vial 2
Vial 2 is missing for injection.

Figure 8 ***Opening the Run Log of a chromatogram file***

CTC Combi PAL Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501494
Revision D

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the Driver 3
    Configuring the Combi PAL 3
    Configuring the Synopsis 5
Building a Method 7
  Creating a New Method 7
  Combi PAL Control Method 9
    Headspace Mode 11
    SPME Mode 12
    Liquid Mode 13
Starting and Viewing an Acquisition 15
  Quick Start and Sequence 15
    Quick Start (Single Acquisition) 15
    Sequence 16
  Running Acquisition Status 16
    Viewing a Running Acquisition 16
    Status of the Combi PAL 16

Introduction

This document describes the configuration of the Combi PAL driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Combi PAL

Click on the button corresponding to the Combi PAL driver and the configuration screen appears.

The toolbar allows you to easily scroll through the configuration windows:

to select the first configuration window.

to select the previous configuration window.

to select the next configuration window.

Configuration Window

Computer Hardware Parameter Group:

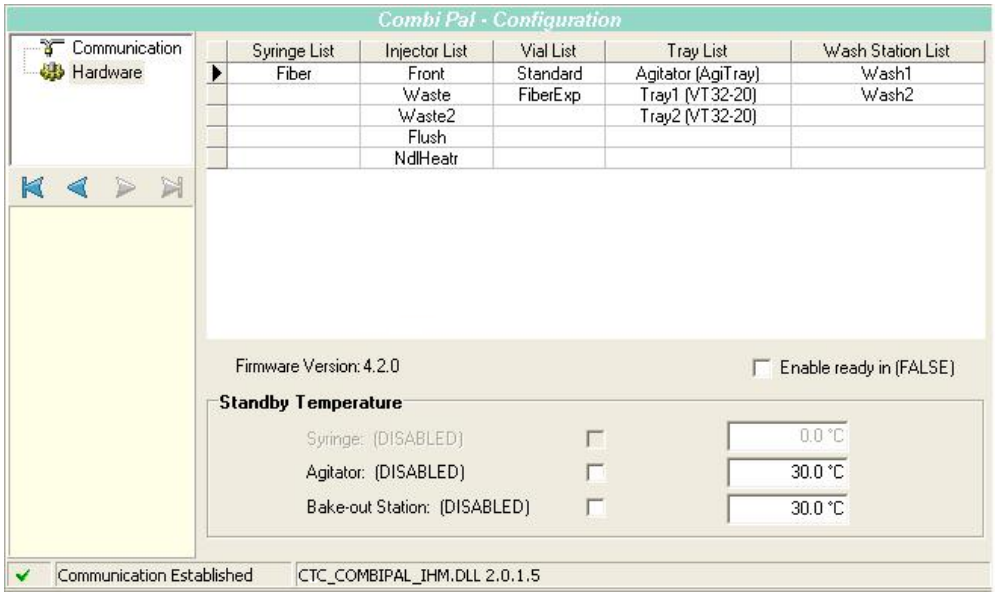
Select the Local Serial Port or the STAR 800 & 850 MIB Serial Port connected to the Combi PAL.

Communication Setup Parameter Group:

Select the corresponding Port Number of the computer.

Once the communication settings have been configured properly, close and reopen the Configure window in order to receive the Combi PAL configuration. The following screen is displayed when downloading the configuration of the Combi PAL.

Hardware Window



Syringe List: Displays the type of syringe installed on the autosampler. More information about the syringe list is displayed in the information field in yellow if the user clicks on the cell.

Injector List: Displays the list of injectors configured on the autosampler. More information about the injector list is displayed in the information field in yellow if the user clicks on the cell.

Vial List: Displays the list of vials configured on the autosampler. More information about the vial list is displayed in the information field in yellow if the user clicks on the cell.

Tray List: Displays the list of trays configured on the autosampler. More information about the tray list is displayed in the information field in yellow if the user clicks on the cell.

Wash Station List: Displays the list of wash stations configured on the autosampler. More information about the wash station list is displayed in the information field in yellow if the user clicks on the cell.

Check or uncheck the Enable ready in to activate or deactivate this option. If it is checked, the Combi PAL waits for a hardware “ready” input signal before starting. A Sync Signal called exactly "READY" must be created in the Combi PAL configuration.

Standby Temperature Parameter Group:

Depending of the Combi PAL configuration, the following standby temperature parameters may be available.

Check or uncheck the Syringe box to activate or deactivate this option. If this option is checked then the standby temperature of the syringe can be entered in the corresponding field.

Check or uncheck the Agitator box to activate or deactivate this option. If this option is checked then the standby temperature of the agitator can be entered in the corresponding field.

Check or uncheck the Bakeout Station box to activate or deactivate this option. If this option is checked then the standby temperature of the Bakeout Station can be entered in the corresponding field.

NOTE: If you want to modify the Combi PAL configuration, you need to setup the Combi PAL directly on the instrument. Refer to the instrument manual for more details.

Configuring the Synopsis

In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

1. To save the configuration of these devices, click on the OK button.

2. Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

3. Go back to the System Configuration screen (Properties wizard). A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, then connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

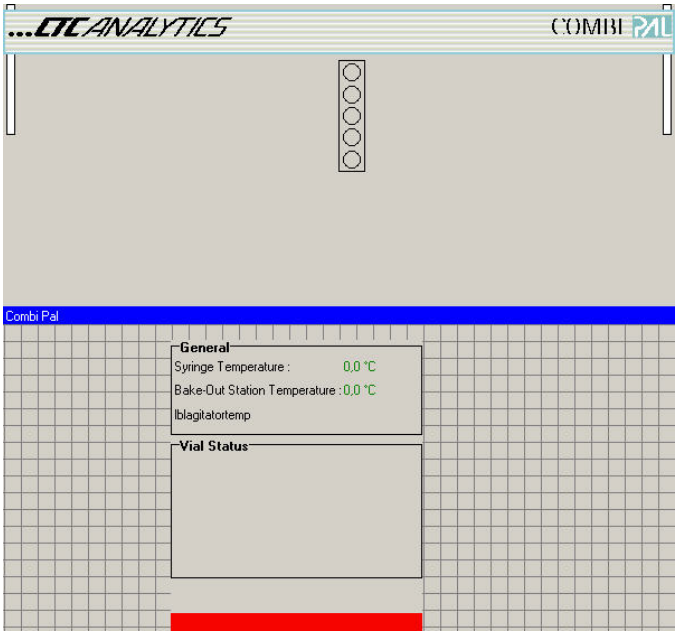
   Click on the to delete a selected tube, click on the buttons to delete all the tubes.

   Click on to define a background color, or on to make the background transparent.

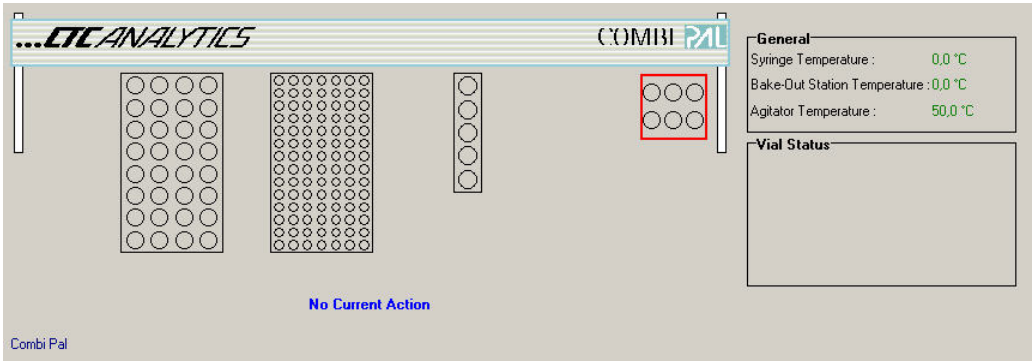
   Click on the icon to change the grid color.

4. Once the synopsis configuration is complete, it will be displayed in CompassCDS, in the Systems tab. In this tab, the Overview part will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.) depending on the installed devices.

For example, the following pictures represent the synopsis of the Combi PAL:



CompassCDS Configuration Manager Screen



CompassCDS Screen

NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Click on the button to print the current configuration.

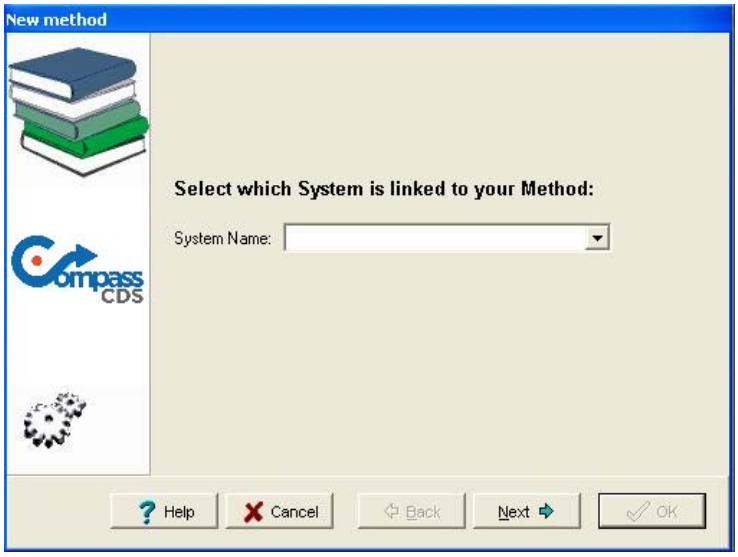
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

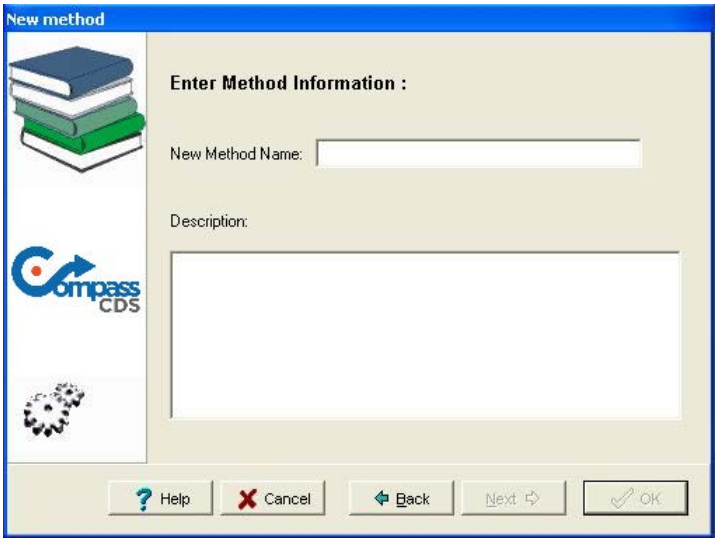
1. To create a new method, select the FILE / NEW METHOD option from CompassCDS main menu.

   A wizard guide will appear and provide assistance during the first steps of method creation:



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

3. Once this field is completed, click on the Next button to move to the second step of the method creation:



4. Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

5. Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in CompassCDS. The next step is the definition of each of the method sections.

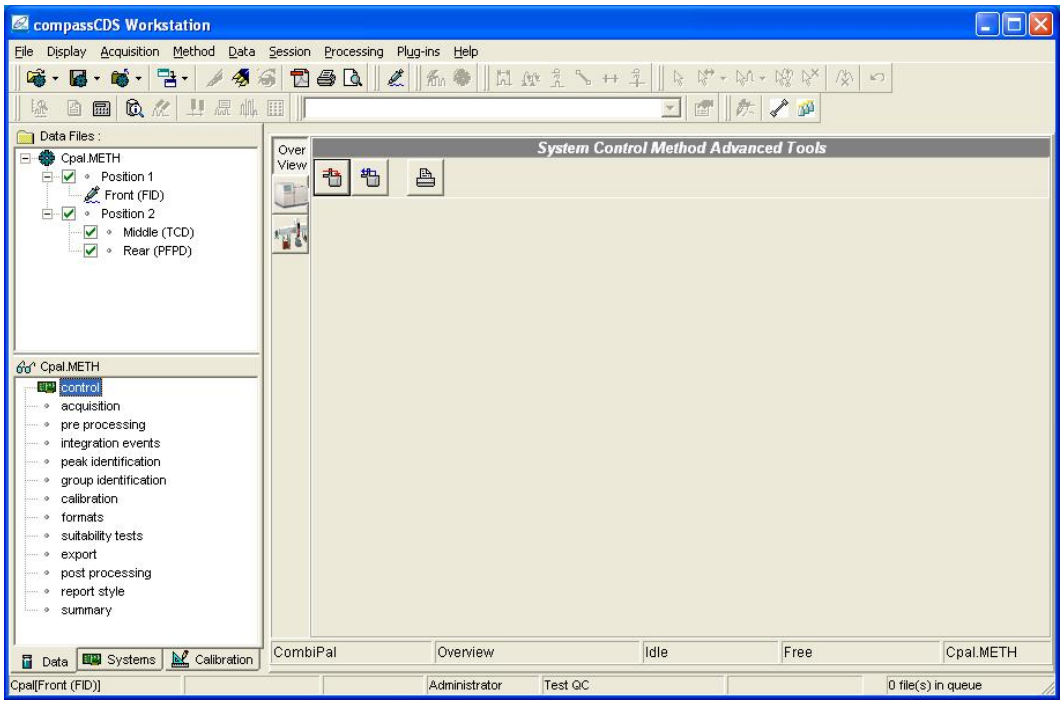
The instrument control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Combi PAL is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to CompassCDS User Guide.

Combi PAL Control Method

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



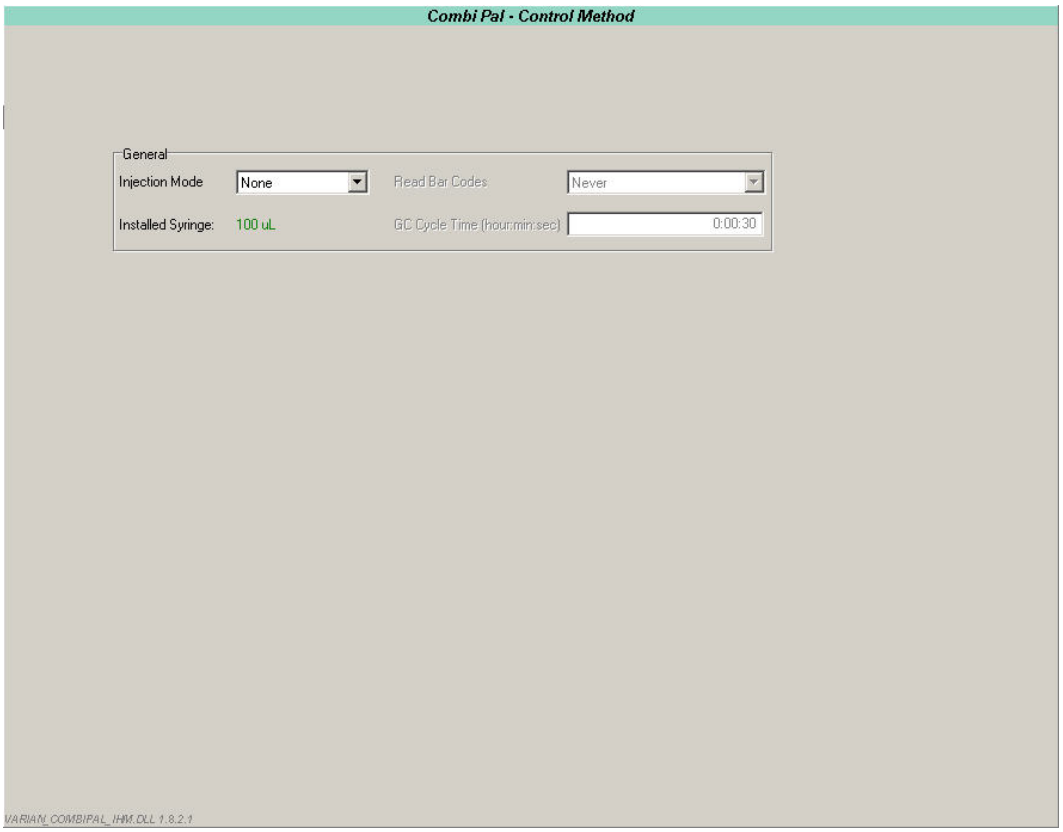
Press the Over View button to display the System Control Method Advanced Tools window:

to send the current method to the instrument.

to get the active method from the instrument.

to print the current method.

Click on the button to display the Combi PAL control method section.



General Parameters Group:

Select the Injection Mode parameters in the scrolling list to specify the injection type made by the autosampler. Four choices are available: None, Liquid, Headspace and SPME. If None is selected the Combi PAL will not perform any injection.

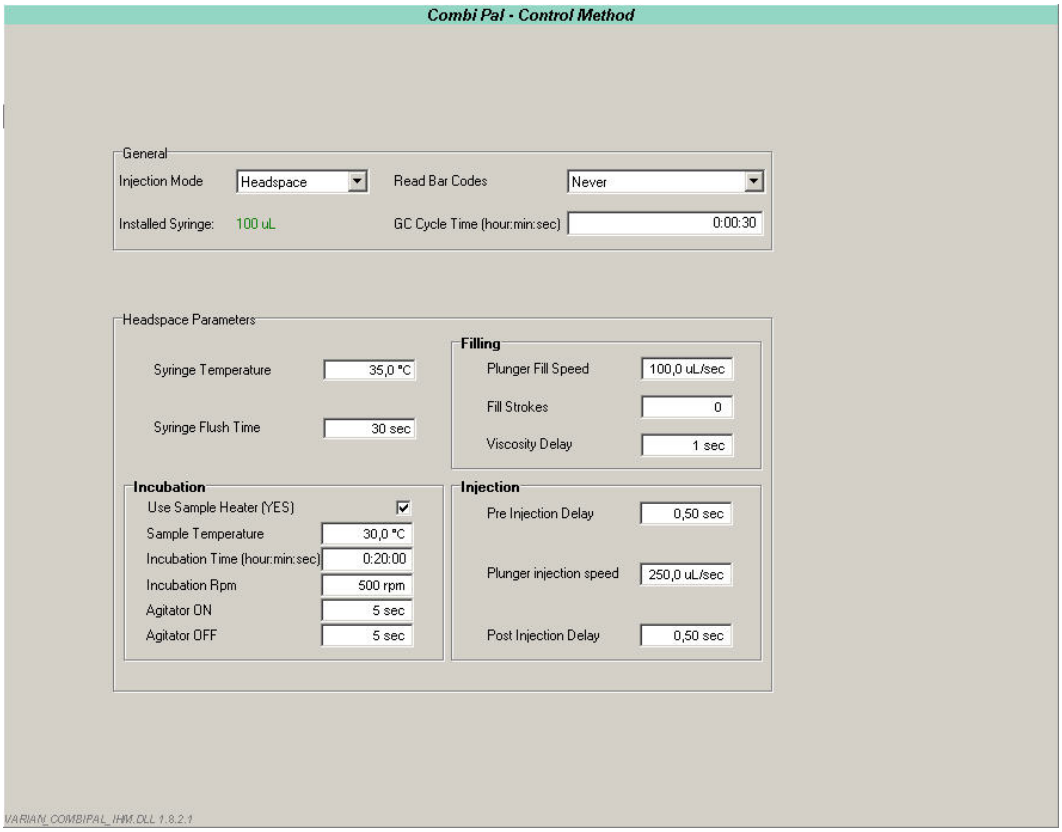
Installed Syringe: It displays the syringe installed on the instrument when the method was created. If the syringe installed on the instrument is different than the one in the method, no run can be performed with that method.

The GC Cycle Time parameter is the total time of an analysis. This parameter is required only if prep-ahead is used.

Select the Read Bar Codes parameters in the scrolling list to specify if and how the Autosampler should use the barcode reader. Three choices are available:

- Never
- For first injection of sample
- For each injection of sample.

Headspace Mode



Syringe Temperature: Specifies the temperature of the syringe if it is heated.

Syringe Flush Time: Specifies the amount of time the syringe will be flushed with gas after the injections.

Incubation Parameters Group:

Check or uncheck the Use Sample Heater box to activate or deactivate the use of the heated agitator.

Sample Temperature: Specifies the temperature of the heated agitator during incubation.

Incubation Time: Specifies the amount of time to heat/agitate the sample before the injection.

Incubation RPM: Specifies the rotation speed for the agitator during incubation.

Agitator On: Specifies the number of seconds the agitator is 'on' during the agitation cycle.

Agitator Off: Specifies the number of seconds the agitator is 'off' during the agitation cycle.

Filling Parameters Group:

Plunger Fill Speed: Sets the speed at which the sample will be drawn up into the syringe.

Fill Strokes: Sets the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.

Viscosity Delay: Specifies the amount of time to wait after drawing up the sample in the syringe to account for the sample's viscosity.

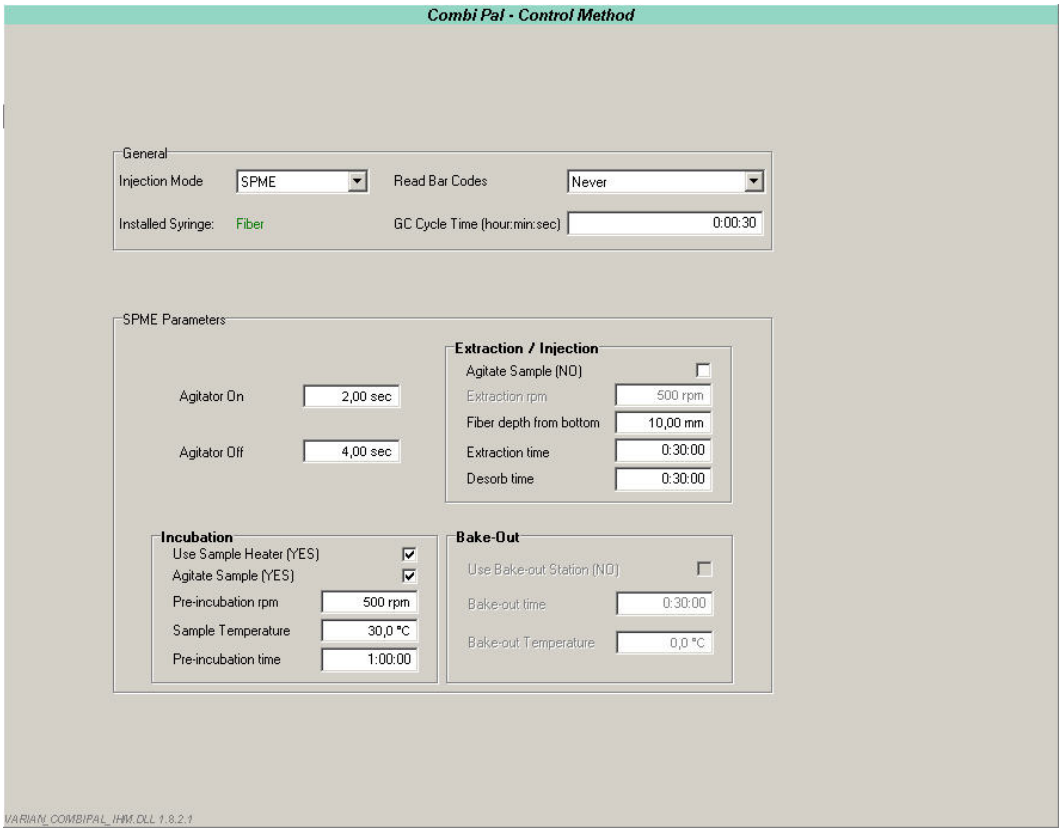
Injection Parameters Group:

Pre Injection Delay: Specifies the amount of time to wait with the needle in the injector before pushing down the plunger.

Plunger Injection Speed: Sets the injection speed.

Post Injection Delay: Specifies the amount of time to keep the syringe in the injector after the injection of sample.

SPME Mode



Agitator On: Specifies the number of seconds the agitator is 'on' during the agitation cycle.

Agitator Off: Specifies the number of seconds the agitator is 'off' during the agitation cycle.

Incubation Parameters Group:

Check or uncheck the Use Sample Heater box to activate or deactivate the use of the heated agitator.

Sample Temperature: Specifies the temperature of the heated agitator during incubation.

Pre-incubation Time: Specifies the amount of time to heat/agitate the sample before the SPME extraction.

Pre-incubation RPM: Specifies the rotation speed for the agitator.

Extraction / Injection Parameters Group:

Fiber depth from bottom: Specifies the height of the fiber's tip above the bottom of the vial.

Extraction RPM: Specifies the rotation speed for the agitator.

Extraction time: Specifies the time the fiber will stay in the sample.

Desorb time: Specifies the time the fiber will be exposed in the injector to desorb the sample.

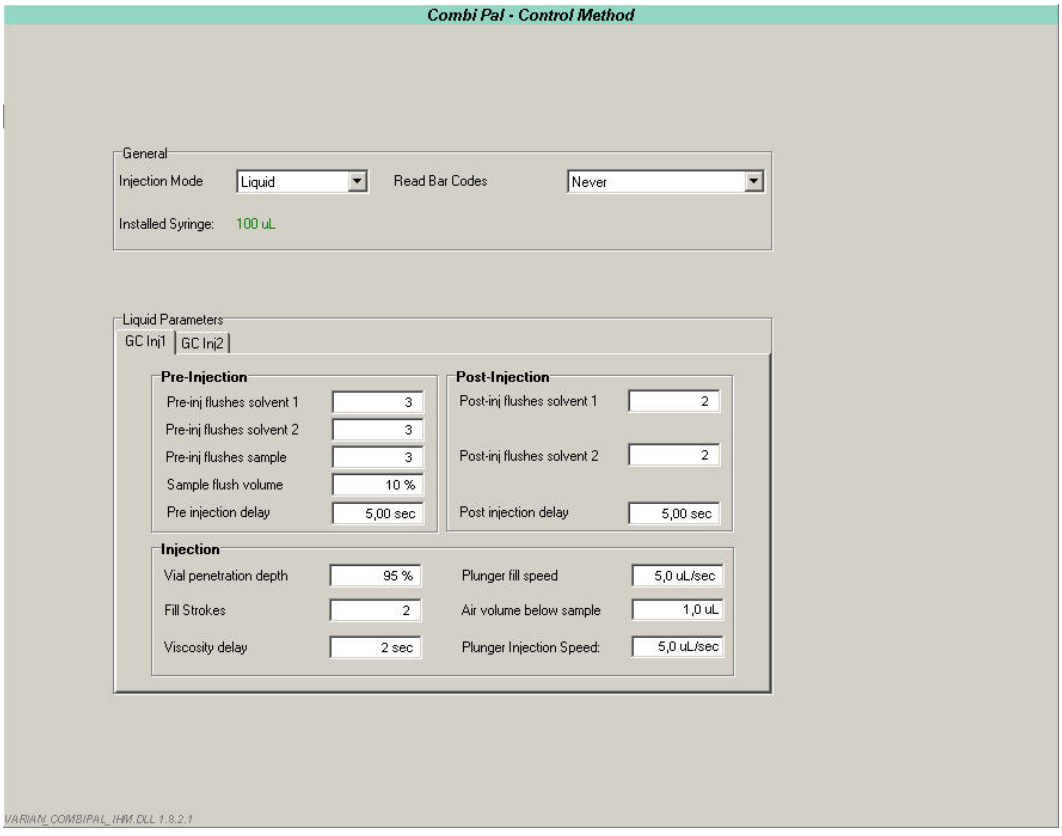
Bake-Out Parameters Group:

Check or uncheck the Use Bake-Out Station box to use or or not the fiber conditioning station to clean the fiber after injection (Yes/No).

Bake-Out temperature: Sets the temperature of the bake-out station where the fiber will be conditioned.

Bake-Out Time: Sets the amount of time to condition the fiber.

Liquid Mode



If multiple injectors are present in the Combi PAL configuration, multiple tabs will appear in the liquid parameters (one tab per injector). Select the tab and define the appropriate injection parameter for each injector.

Pre Injection Parameters Group:

Pre-Inj Flushes Solvent 1: Sets the number of times solvent 1 will be drawn up into the syringe and expelled into the waste vial before flushing with solvent 2.

Pre-Inj Flushes Solvent 2: Sets the number of times solvent 2 will be drawn up into the syringe and expelled into the waste vial before flushing with the sample.

Pre-Inj Flushes Sample: Sets the number of times the sample will be drawn up into the syringe and expelled into the waste vial before injection.

Sample Flush Volume: Specifies the percentage of syringe to be used in sample flushes.

Pre Injection Delay: Specifies the amount of time to wait with the needle in the injector before pushing down the plunger.

Injection Parameters Group:

Vial Penetration Depth: Sets how far the syringe needle goes down into the sample vial. 100% corresponds to the bottom of the vial.

Fill Strokes: Sets the number of times the sample will be pumped in and out of the syringe before loading the sample volume into the syringe.

Viscosity Delay: Specifies the amount of time to wait after drawing up the sample in the syringe to account for the sample's viscosity.

Plunger Fill Speed: Sets the speed at which the sample will be drawn up into the syringe.

Air Volume Below Sample: Specifies the volume of the air gap to draw in after drawing the sample.

Plunger Injection Speed: Sets the injection speed.

Post Injection Parameters Group:

Post Injection Flush 1: Sets the number of times solvent 1 will be drawn up into the syringe and expelled into the waste vial before flushing with solvent 2.

Post Injection FIush 2: Sets the number of times solvent 2 will be drawn up into the syringe and expelled into the waste vial.

Post Injection Delay: Specifies the amount of time to keep the syringe in the injector after the injection of sample.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

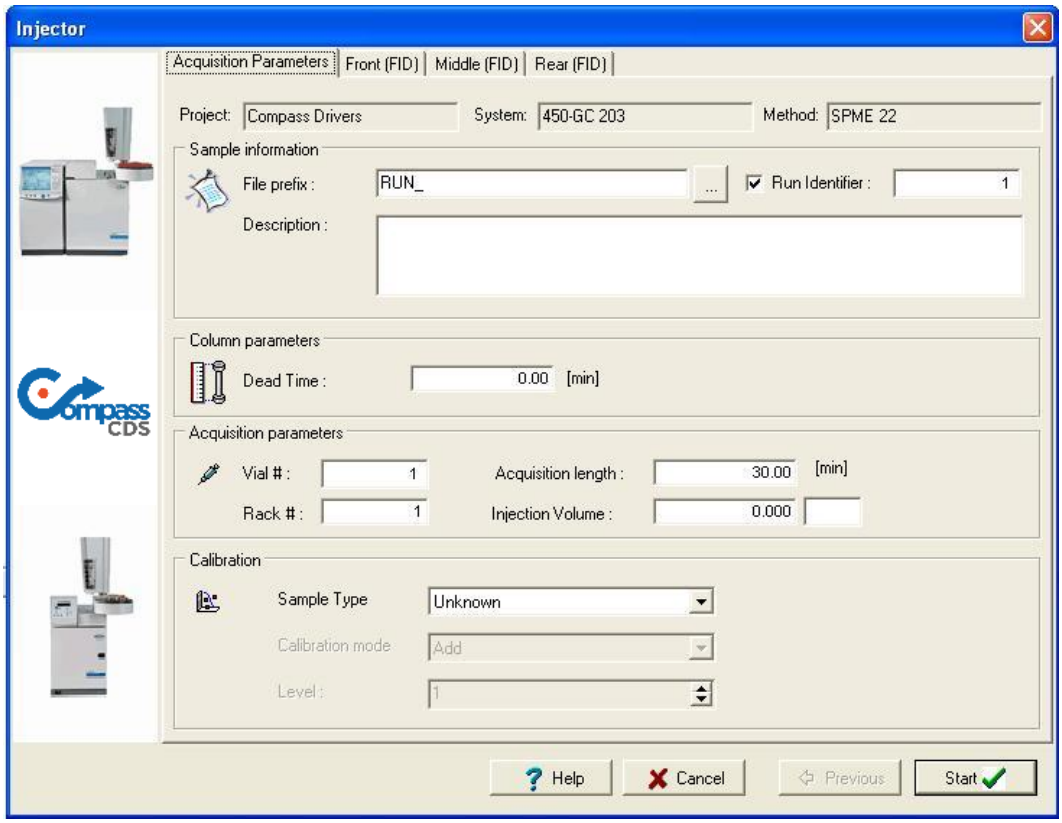
Quick Start (Single Acquisition)

1. Press the button.

   In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

2. Press the OK button.

The following screen is displayed:



In the Acquisition Parameters tab, required fields like the Run Name, the Run ID and the Acquisition length must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by CompassCDS, the Injection Volume, the Vial position and the Rack number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the Channel X tab.

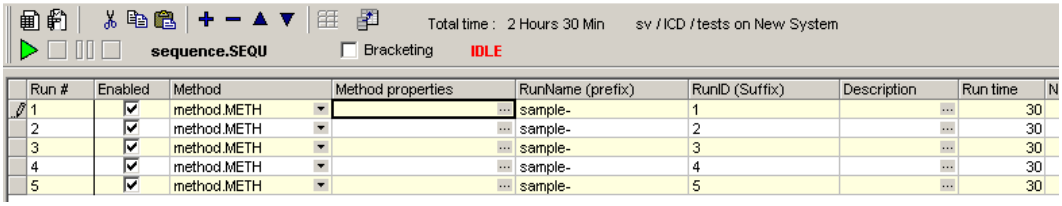
3. Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple

injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time	N
1	☑	method.METH		sample-	1		30	
2	☑	method.METH		sample-	2		30	
3	☑	method.METH		sample-	3		30	
4	☑	method.METH		sample-	4		30	
5	☑	method.METH		sample-	5		30	

The Method Name, the Run Name, the Run ID, and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to CompassCDS User Guide.

Running Acquisition Status

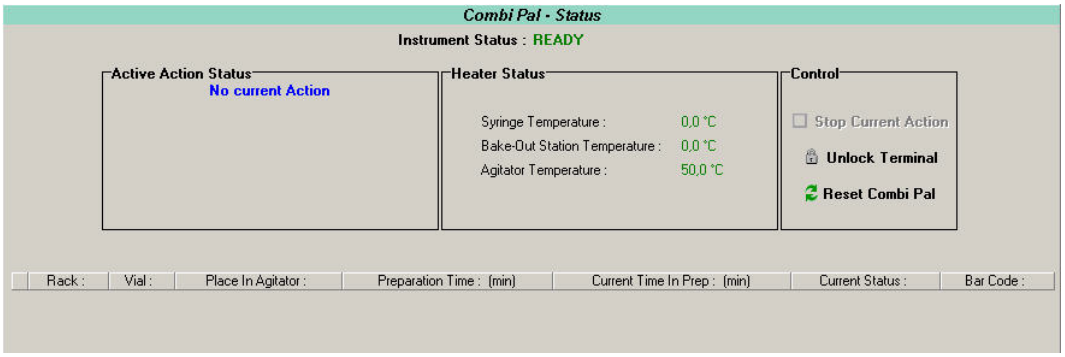
Viewing a Running Acquisition

To view a running acquisition, click on the Systems tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Combi PAL

Click on the button corresponding to the Combi PAL driver and the Combi PAL status screen will appear.

Status Window



Instrument Status: This displays the state of the instrument ready or not ready

Active ActionStatus: This displays the action currently done by the Combi PAL

Heater Status Parameter Group:

Syringe Temperature: This parameter displays the current temperature of the syringe if it is a heated syringe.

BakeOut Station Temperature: This parameter displays the current temperature of the bake out station.

Agitator Temperature: This parameter displays the current temperature of the agitator.

Control Buttons

This button stops the current action of the Combi PAL.

This button unlocks the Combi PAL terminal.

This button resets the Combi PAL.

The table in the status displays what vials are used by the Combi PAL and their state.

Rack: This parameter indicates the rack of the vial

Vial: This parameter indicates the position of the vial

Place in agitator: This parameter indicates the position the vial in the agitator.

Preparation Time: This parameter shows how long the vial will be prepared and the current preparation time.

Actual time in prep: This parameter gives the current preparation time.

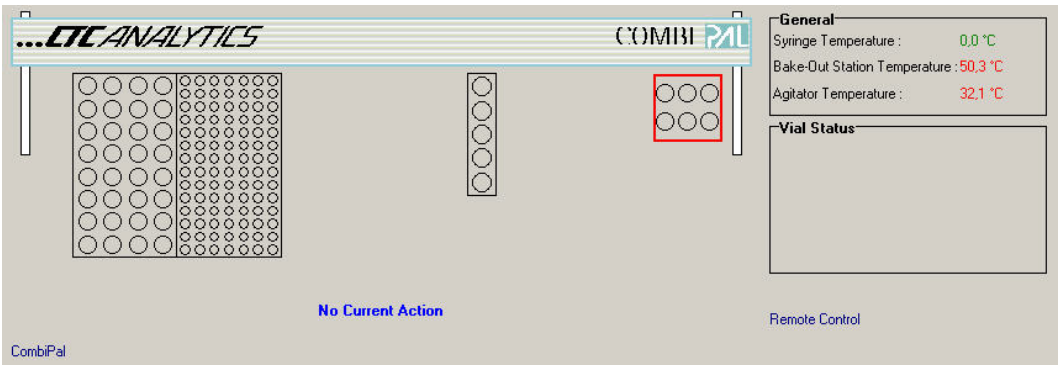
Actual Status: This parameter gives the status of the vial. It can be transport, preparation, ready, injecting and injected.

Bar code: This parameter displays if the bar code of the vial.

Overview Window

Click on the Over View button: the Status Overview window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (temperatures and pressures).



Not Ready: contains the not ready information sent by the instrument.

Events: contains the events that have occurred on the instrument.

Valco® Valve Control Driver
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501595
Revision D

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the Driver 3
    Configuring the Valco valve driver 3
    Configuring the Synopsis 4
Building a Method 6
  Creating a New Method 6
  Control Method Section for the Valco Valve 8
Starting and Viewing an Acquisition 10
  Quick Start and Sequence 10
    Quick Start (Single Acquisition) 10
  Running Acquisition Status 11
    Viewing a Running Acquisition 11
    Status of the Valco Valve 11
Appendix 13
  Stream Selection 13
  VICI Valve Configurator 16

Introduction

This document describes the configuration of the Valco® valve driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS Installation Guide.

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Valco valve driver

Click on the button corresponding to the Valco valve driver and the configuration screen appears.

The toolbar allows you to easily scroll through the configuration windows:

to select the first configuration window.

to select the previous configuration window.

to select the next configuration window.

to select the final configuration window.

Communication Window

Communication Setup parameter group:

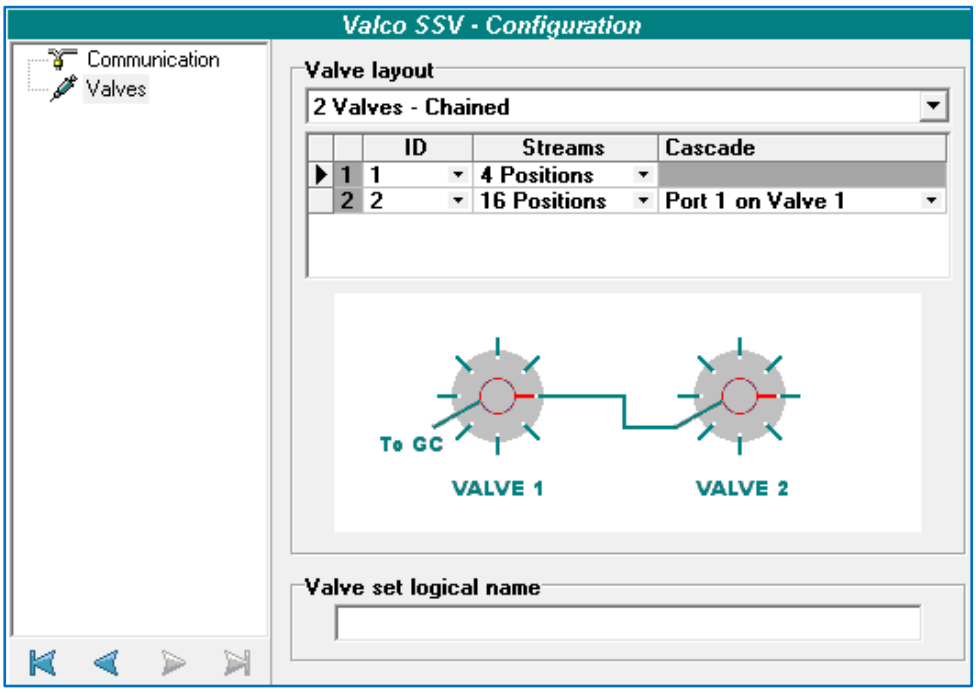
Select whether the instrument is connected to a Local Serial Port, a Varian CP-3800 Serial Integrated Device, or a STAR 800 & 850 MIB serial port.

Select the corresponding Port number where the instrument is connected.

Select the Baud Rate of the Valve according to the instrument configuration.

NOTE: To configure the Baud Rate and ID of a Valco Valve, use the VICI Valve configurator tool. Please refer to the appendix VICI Valve Configurator on page 16 for more details.

Valves Window



Valve layout parameter group:

Select the number of valve connected to the system and then for each valve, configure its ID, its number of Streams and, if required, its Cascade position.

Enter a logical name for the Valve system if required. This can be useful when two systems of valves are connected on a multi-injector GC, in order to differentiate them.

NOTE: Depending on the valve layout, the way to select the valve stream in the method will change. Please refer to the appendix Stream Selection on page 13 for more details.

NOTE: To configure the Baud Rate and ID of a Valco Valve, use the VICI Valve configurator tool. Please refer to the appendix VICI Valve Configurator on page 16 for more details.

Configuring the Synopsis

In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

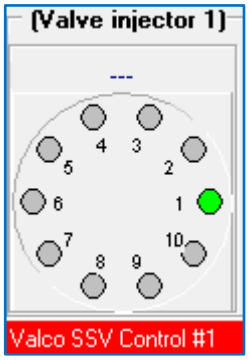
1. To save the configuration of these devices, click on the OK button.
2. Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

3. Go back to the System Configuration screen (Properties wizard). A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, then connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

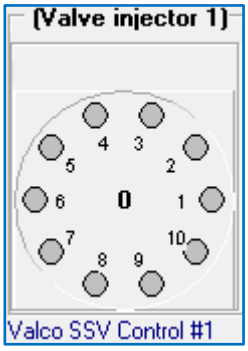
   Click on to delete a selected tube, click on the buttons to delete all the tubes.
   Click on to define a background color, or on to make the background transparent.
   Click on the icon to change the grid color.

4. Once the synopsis configuration is complete, it will be displayed in CompassCDS, in the Systems view, accessed from the Systems tab. In this view, the Overview section shows the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.) depending on the installed devices.

   For example, the following pictures represent the overview of the Valco Valve:



CompassCDS Configuration Manager Screen



CompassCDS Screen

NOTE: Once the system has been created and correctly configured, it must be associated with one or more CompassCDS Projects in order to start data acquisition. For more information on the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Click on the button to print the current configuration.

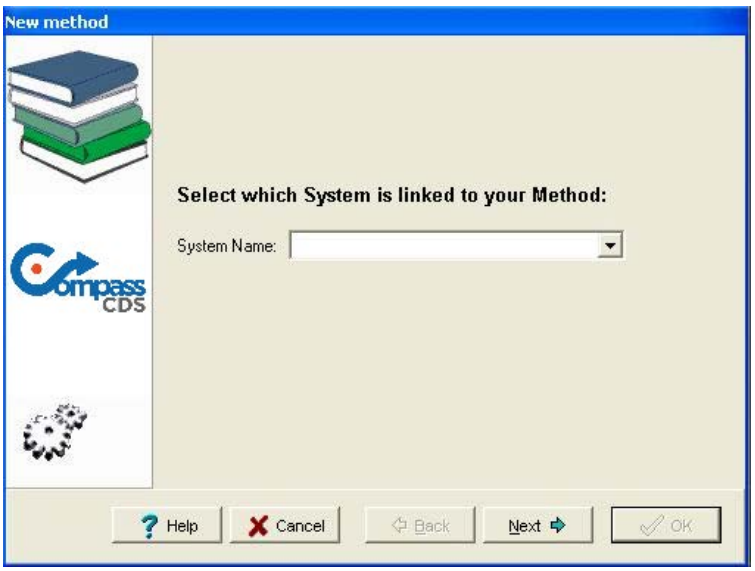
Building a Method

Creating a New Method

The CompassCDS method tree contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the method tree sub-sections; however, the instrument control and acquisition sections must be completed in order to start acquiring data.

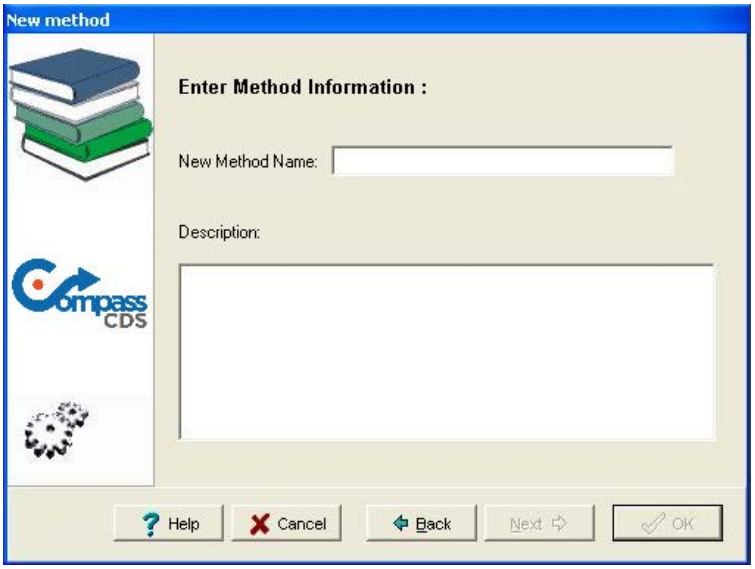
1. To create a new method, select the FILE / NEW METHOD option from CompassCDS main menu.

   A method creation wizard guides users through the initial steps of method creation:



2. Select the system (chromatograph) to be associated with the method. CompassCDS methods are created for particular systems and only methods associated with that system will be available for selection during data acquisition.

3. Once this field has been completed, click on the Next button to move to the second step of the method creation wizard:



4. Enter the New Method Name in the first field. Information concerning the method can be entered into the optional Description field.

5. Once these fields have been completed, click on the OK button. The new method is created and is opened with default parameters in CompassCDS. The next step is the definition of each of the method tree sections.

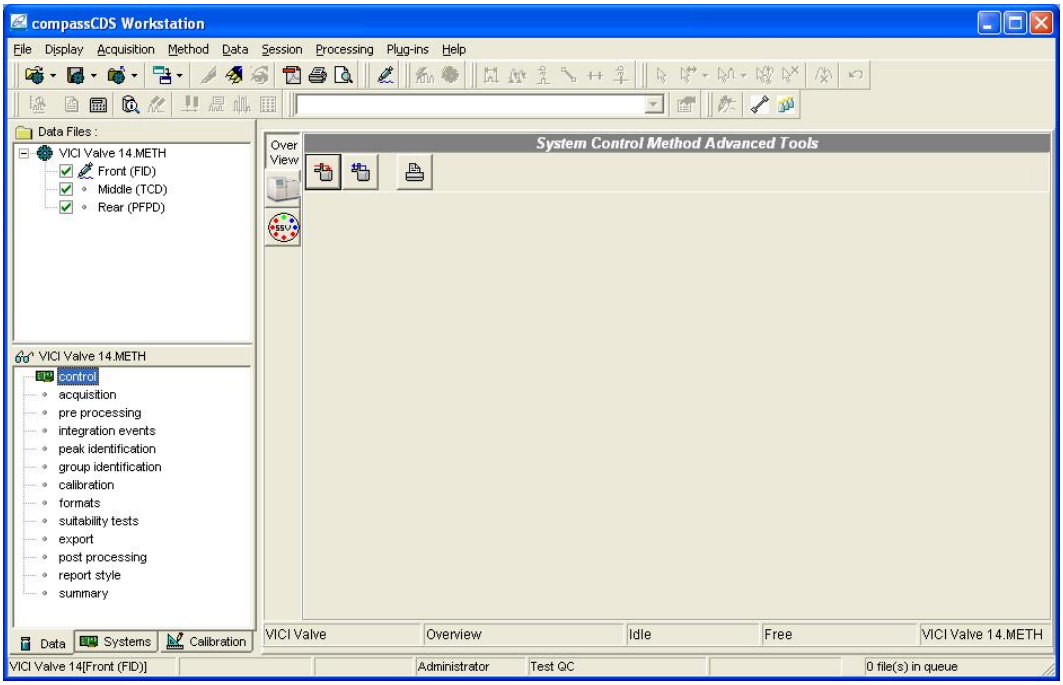
   The instrument control and acquisition section must be defined in order to start an acquisition. In the following section of this guide, only the instrument control section for the Valco Valve is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more information on the programming of each method section, refer to the CompassCDS User Guide.

Control Method Section for the Valco Valve

Once the new method is created, select the control section in the lower part of the browser (method tree).

The following screen appears:



Press the Over View button to display the System Control Method Advanced Tools window:

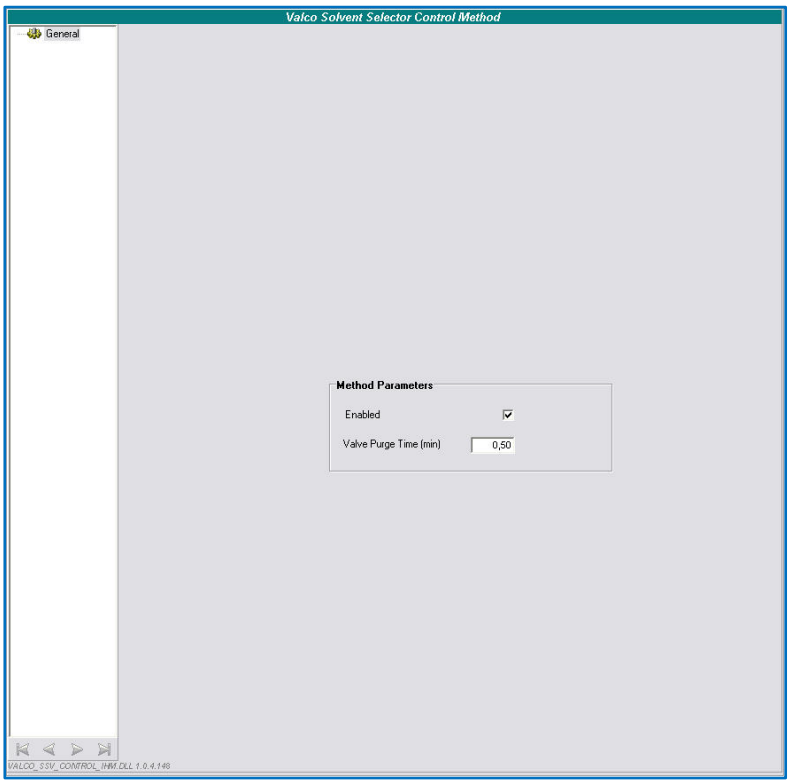
to send the current method to the instrument.

to get the active method from the instrument.

to print the current method.

Click on the button to display Valco valve control method section. It contains one sub-section: Parameters.

General Control



Method parameter group

Enable: Check or uncheck this feature to use or not to use the Valco injector.

NOTE: Other ways to disable the Valco injector are:

- - Enter 0 as the vial number in the Valco acquisition parameters (see the Starting and Viewing an Acquisition section).
- - Uncheck the Valco injector in the method.

Enter the Valve Purge Time in the corresponding field.

NOTE: Depending of the valve layout, the way to select the valve stream in the method will change. Please refer to the appendix Stream selection for more details.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

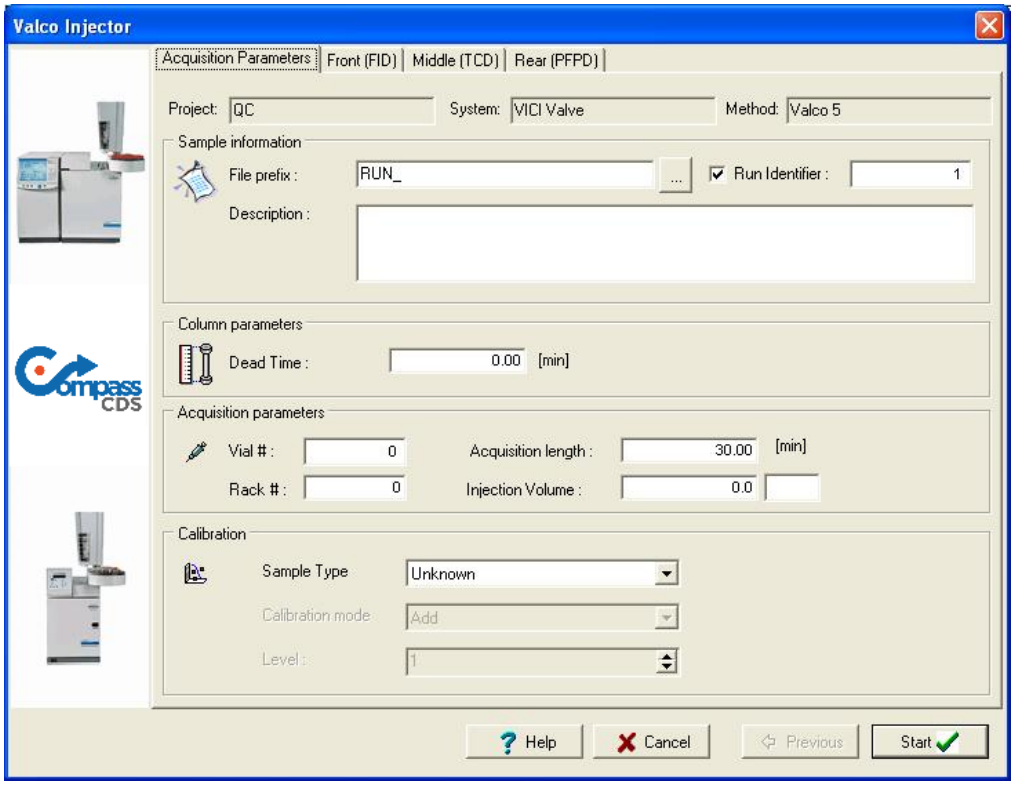
Quick Start (Single Acquisition)

1. Press the button.

   In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

2. Press the OK button.

   The following screen is displayed:



   In the Acquisition Parameters tab, required fields like the Run Name, the Run ID and the Acquisition length must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by CompassCDS, the Injection Volume, the Vial position and the Rack number (if required) must be entered.

   Other parameters associated with each acquisition channel can be entered in the Channel X tab.

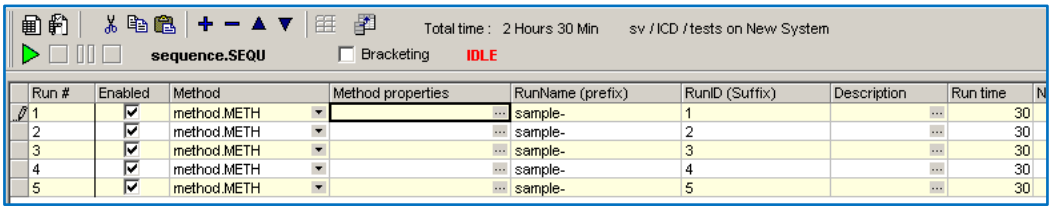
3. Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple

injector system, the same parameters entered for the first injector must be entered for additional injectors before starting the acquisition.

Sequence

1. To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to CompassCDS User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to CompassCDS User Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time
1	☑	method.METH		sample-	1		30
2	☑	method.METH		sample-	2		30
3	☑	method.METH		sample-	3		30
4	☑	method.METH		sample-	4		30
5	☑	method.METH		sample-	5		30

The Method Name, the Run Name, the Run ID, and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

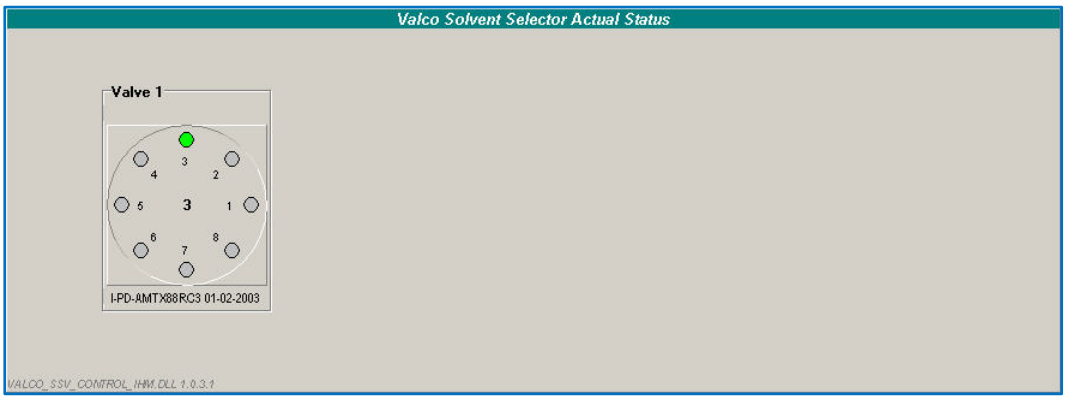
To view a running acquisition, click on the Systems tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Valco Valve

Click on the

button corresponding to the Valco Valve driver and the Valco Valve status screen will appear.

Status Window

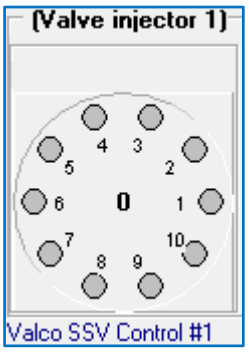


This screen displays the position of each valve. If the system is idle change the stream position by clicking on the desired position.

Overview Window

Click on the Over View button: the Status Overview window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where the current valve position can be read. If the system is idle change the stream position by clicking on the desired position.



Not Ready: contains the not ready information sent by the instrument.

Events: contains the events that have occurred on the instrument.

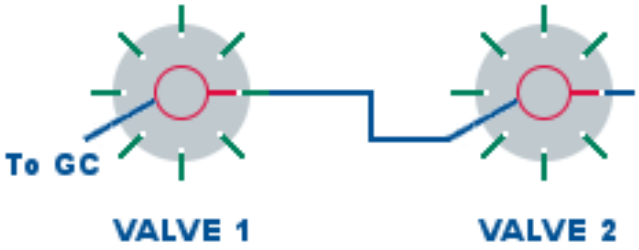
Appendix

Stream Selection

1 Valve

In this case, enter the stream number in the vial field.

2 Valves Chained



In this case, enter the stream number in the vial field. Each stream will have a unique number from 1 to the sum of valve 1 ports and valve 2 ports. The port of valve 1 where the valve 2 is cascaded will be automatically selected when injecting from a stream on valve 2.

Examples

If the user wants to select the stream 2 of valve 1, the value to enter in the vial field will be 2.

If the user wants to select the stream 5 of the valve 2 and valve 1 has 16 positions, the value to enter in the vial field is 5+16=21

3 Valves Chained

In this case, enter the stream number in the vial field. Each stream will have a unique number from 1 to the sum of valve 1 ports, valve 2 ports and valve 3 ports. The port of valve 1 where the valve 2 is cascaded will be automatically selected when injecting from a stream on valve 2 or 3. The port of valve 2 where the valve 3 is cascaded will be automatically selected when injecting from a stream on valve 3.

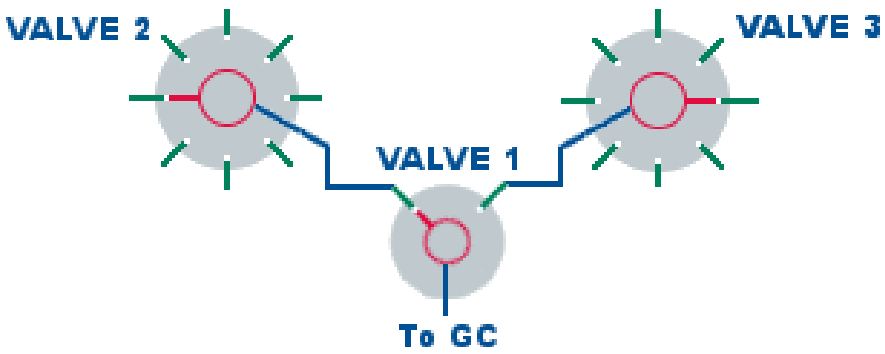
Examples

If the user wants to select the stream 2 of valve 1, the value to enter in the vial field will be 2.

If the user wants to select the stream 5 of the valve 2 and valve 1 has 16 positions, the value to enter in the vial field is 5+16=21

If the user wants to select the stream 8 of valve 3 and valve 1 and 2 have 10 positions, the value to enter in the vial field is 8+10+10=28

3 Valves Networked



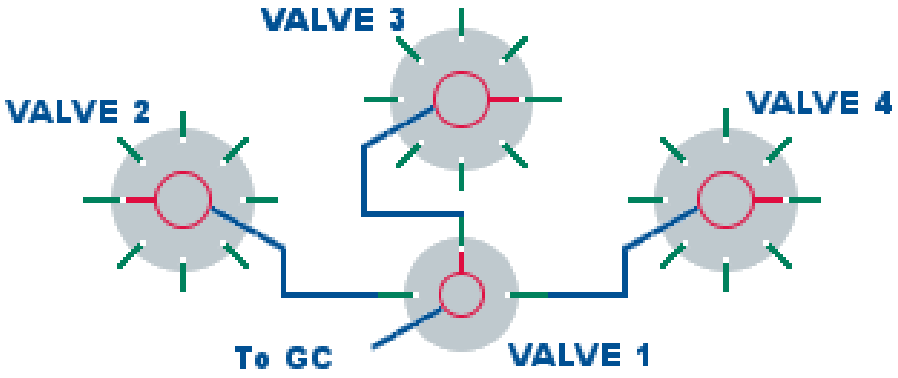
In this case, enter the stream number of valve 1 in the rack field and the stream number of valve 2 or 3 in the vial field.

Examples

If the user wants to select the stream 5 of the valve 2 and valve 2 is connected to the stream 1 of Valve 1, the value to enter in the vial field is 5 and in the rack field 1

If the user wants to select the stream 6 of the valve 3 and valve 3 is connected to the stream 2 of Valve 1, the value to enter in the vial field is 6 and in the rack field 2

4 Valves Networked



In this case, enter the stream number of valve 1 in the rack field and the stream number of valve 2, 3 or 4 in the vial field.

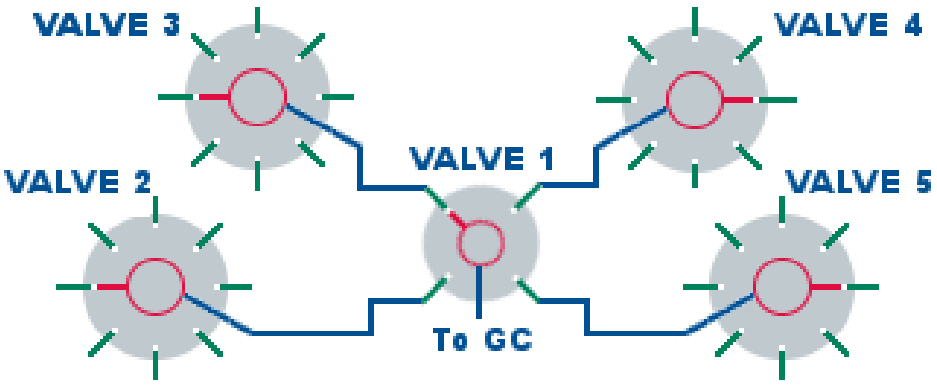
Examples:

If the user wants to select the stream 5 of the valve 2 and valve 2 is connected to the stream 1 of Valve 1, the value to enter in the vial field is 5 and in the rack field 1

If the user wants to select the stream 6 of the valve 3 and valve 3 is connected to the stream 2 of Valve 1, the value to enter in the vial field is 6 and in the rack field 2

If the user wants to select the stream 11 of the valve 4 and valve 4 is connected to the stream 3 of Valve 1, the value to enter in the vial field is 11 and in the rack field 3

5 Valves Networked:



In this case, enter the stream number of valve 1 in the rack field and the stream number of valve 2, 3, 4 or 5 in the vial field.

Examples:

If the user wants to select the stream 5 of the valve 2 and valve 2 is connected to the stream 1 of Valve 1, the value to enter in the vial field is 5 and in the rack field 1

If the user wants to select the stream 6 of the valve 3 and valve 3 is connected to the stream 2 of Valve 1, the value to enter in the vial field is 6 and in the rack field 2

If the user wants to select the stream 11 of the valve 4 and valve 4 is connected to the stream 3 of Valve 1, the value to enter in the vial field is 11 and in the rack field 3

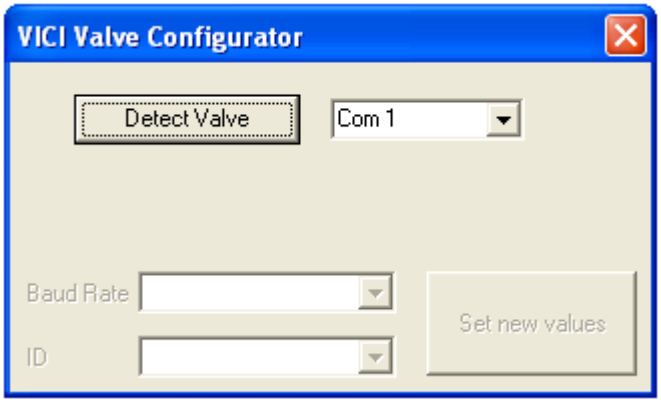
If the user wants to select the stream 15 of the valve 5 and valve 5 is connected to the stream 4 of Valve 1, the value to enter in the vial field is 15 and in the rack field 4

VICI Valve Configurator

The VICI Valve Configurator is a tool to configure the baud rate and the ID of the VICI Valves.

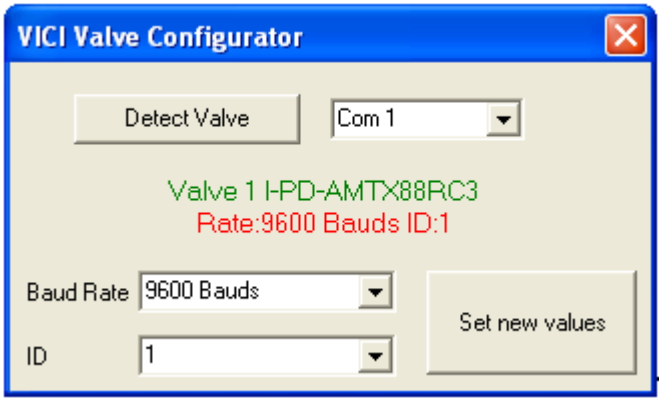
To configure a valve, follow the steps described below:

1. Connect the valve to a COM port of the local computer.
2. Launch the executable file called "VICI_CONF_VALVE.EXE" located in the CompassCDS\Server folder.
3. The following window will appear



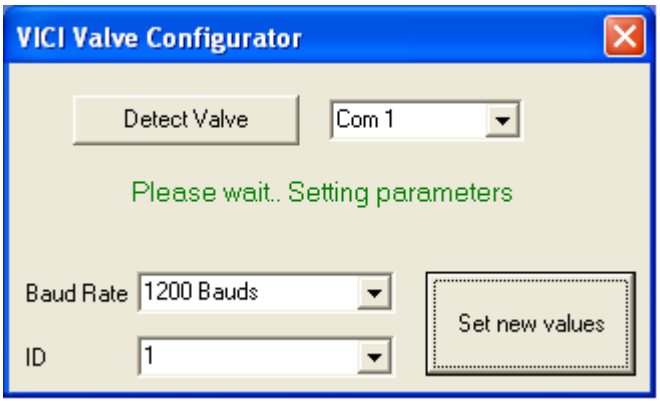
4. Select on which COM port the valve is connected and press the button

5. The valve will be automatically detected and its current Baud rate and ID parameter will be displayed as below.

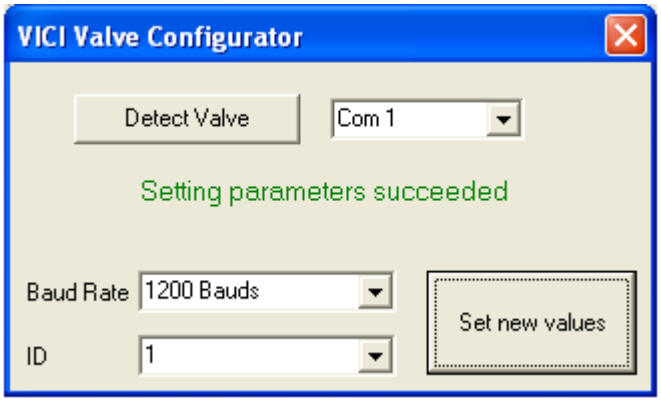


6. Change the Baud Rate and/or the ID value and press the

button, the following screen will be displayed.



6. Once the parameters are correctly set in the valve, the following confirmation message will be displayed.



National Instruments
NI-9219 A/D Converter (ADC) Interface
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501590
Revision C

Contents

Introduction 3
NI-DAQMX Software Installation 4
Configuring the NI-9184 Ethernet Chassis Hostname and IP Address using the NI-DAQMX Software 6
Connecting the NI-9219 ADC Module 10
Connecting the NI-9401 TTL I/O Module as the Start In device for the NI-9219 ADC 11
Installing the National Instruments Control Drivers and Configuring a System in Configuration Manager 13
Creating a Method in CompassCDS 17
Adding the NI-9481 Relay Module as an additional module in the NI-9184 Chassis 19
NI Modules - Technical Specifications 22
  NI-9184 Chassis 22
  NI-9219 ADC Module 22
  NI-9401 TTL I/O Module 23

Introduction

When analog data acquisition from GC/LC instruments into CompassCDS is a requirement, this can be done using the National Instruments 9219 ADC Module installed together with the NI-9401 TTL I/O module in the NI-9184 4 slot Ethernet chassis. These modules are shown below. It is also possible to add the NI-9841 Relay module as an optional unit when contact closure relay functionality is required.

NI-9184 4-slot Ethernet Chassis

NI-9219 4-Channel Analog to Digital converter module

NI-9401 TTL I/O module

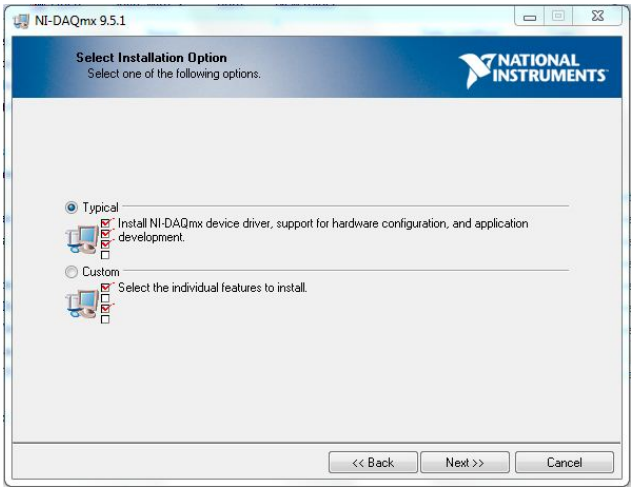
NI-9924 Terminal Connector

NI-9481 4-Channel Relay module (Optional)

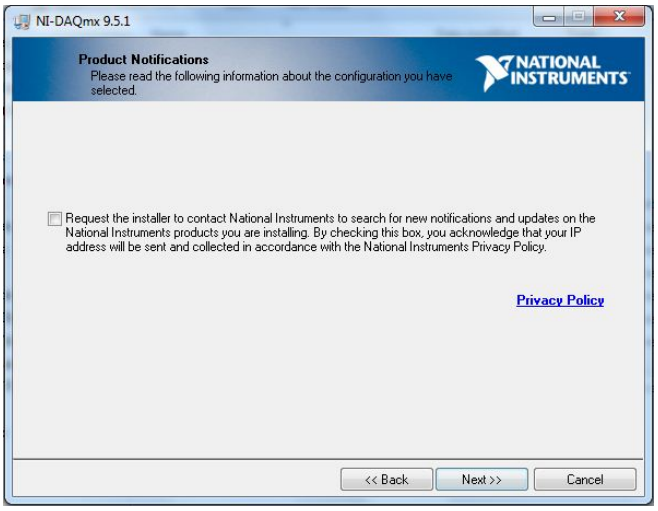
NI-DAQMX Software Installation

The NI-DAQMX software supplied with the NI-9184 Chassis is required to be installed in order to configure the NI-Modules as described in this user guide. Configuration includes assigning a unique hostname, a static IP address, a subnet mask and if required a Gateway IP. This software is installed from the vendor supplied NI-DAQMX DVD as follows:

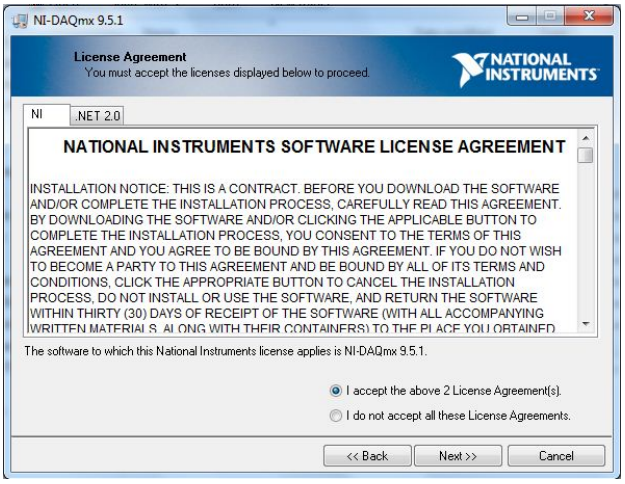
1. Select the Typical installation option and click Next.



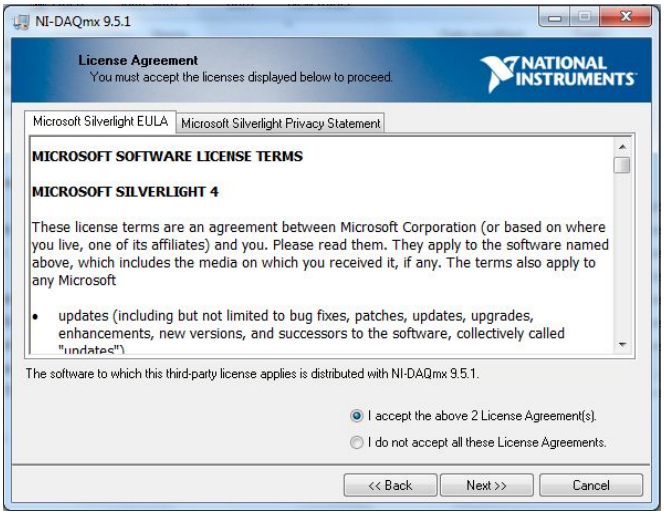
2. Uncheck the “Request the installer to contact National Instruments” option and click Next.


NI-DAQmx 9.5.1
Product Notifications
Please read the following information about the configuration you have selected.
NATIONAL INSTRUMENTS
Request the installer to contact National Instruments to search for new notifications and updates on the National Instruments products you are installing. By checking this box, you acknowledge that your IP address will be sent and collected in accordance with the National Instruments Privacy Policy.
Privacy Policy
<< Back
Next >>
Cancel

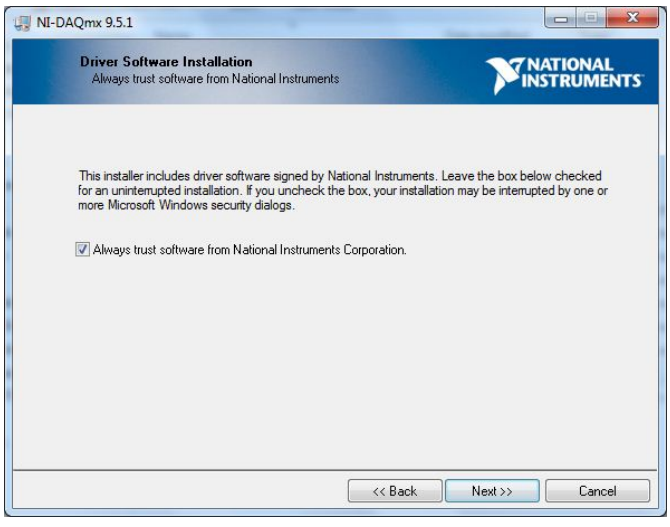
3. Accept the National Instruments license agreements and click Next.


NI-DAQmx 9.5.1
License Agreement
You must accept the licenses displayed below to proceed.
NATIONAL INSTRUMENTS
NI
.NET 2.0
NATIONAL INSTRUMENTS SOFTWARE LICENSE AGREEMENT
INSTALLATION NOTICE: THIS IS A CONTRACT. BEFORE YOU DOWNLOAD THE SOFTWARE AND/OR COMPLETE THE INSTALLATION PROCESS, CAREFULLY READ THIS AGREEMENT. BY DOWNLOADING THE SOFTWARE AND/OR CLICKING THE APPLICABLE BUTTON TO COMPLETE THE INSTALLATION PROCESS, YOU CONSENT TO THE TERMS OF THIS AGREEMENT AND YOU AGREE TO BE BOUND BY THIS AGREEMENT. IF YOU DO NOT WISH TO BECOME A PARTY TO THIS AGREEMENT AND BE BOUND BY ALL OF ITS TERMS AND CONDITIONS, CLICK THE APPROPRIATE BUTTON TO CANCEL THE INSTALLATION PROCESS, DO NOT INSTALL OR USE THE SOFTWARE, AND RETURN THE SOFTWARE WITHIN THIRTY (30) DAYS OF RECEIPT OF THE SOFTWARE (WITH ALL ACCOMPANYING
The software to which this National Instruments license applies is NI-DAQmx 9.5.1.
I accept the above 2 License Agreement(s).
I do not accept all these License Agreements.
<< Back
Next >>
Cancel

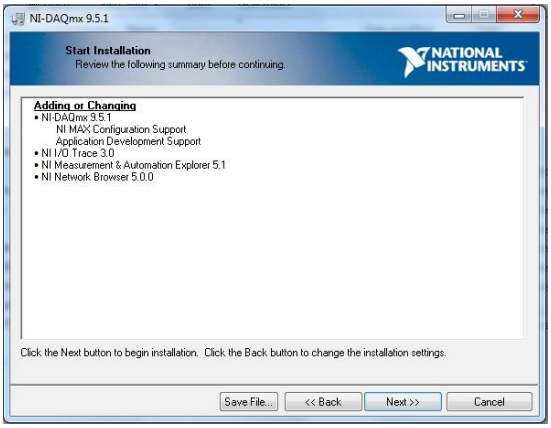
4. Accept the Microsoft software licenses and click Next.

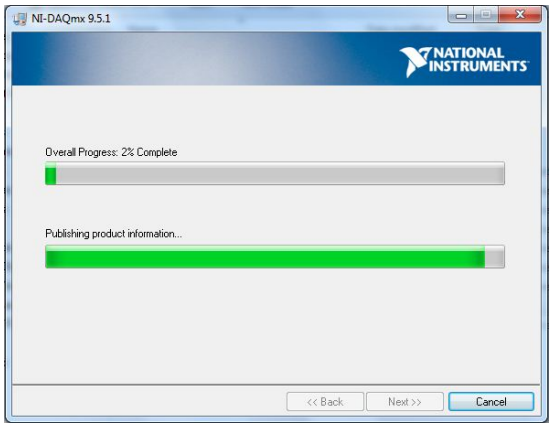

NI-DAQmx 9.5.1
License Agreement
You must accept the licenses displayed below to proceed.
NATIONAL INSTRUMENTS
Microsoft Silverlight EULA
Microsoft Silverlight Privacy Statement
MICROSOFT SOFTWARE LICENSE TERMS
MICROSOFT SILVERLIGHT 4
These license terms are an agreement between Microsoft Corporation (or based on where you live, one of its affiliates) and you. Please read them. They apply to the software named above, which includes the media on which you received it, if any. The terms also apply to any Microsoft
updates (including but not limited to bug fixes, patches, updates, upgrades, enhancements, new versions, and successors to the software, collectively called
The software to which this third-party license applies is distributed with NI-DAQmx 9.5.1.
I accept the above 2 License Agreement(s).
I do not accept all these License Agreements.
<< Back
Next >>
Cancel

5. Check the “Always trust software from National Instruments Corporation” option and click Next.

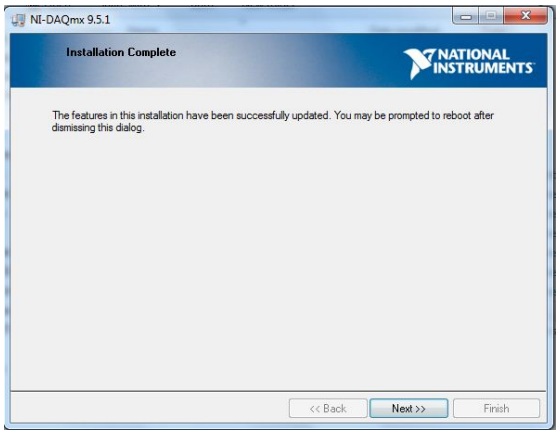

NI-DAQmx 9.5.1
Driver Software Installation
Always trust software from National Instruments
NATIONAL INSTRUMENTS
This installer includes driver software signed by National Instruments. Leave the box below checked for an uninterrupted installation. If you uncheck the box, your installation may be interrupted by one or more Microsoft Windows security dialogs.
Always trust software from National Instruments Corporation.
<< Back
Next >>
Cancel

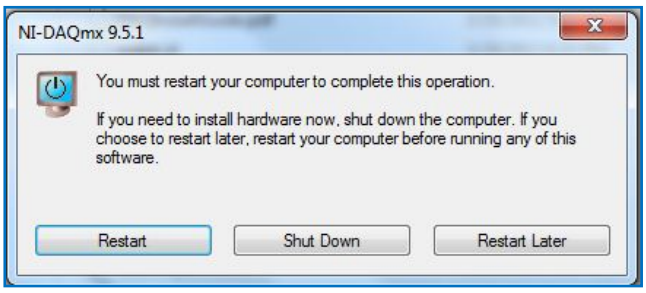
6. Click the Next button to start the installation. The installation of this software can take 20-30 minutes. The progress bar (shown below) indicates the state of the installation.


NI-DAQmx 9.5.1
Start Installation
Review the following summary before continuing.
NATIONAL INSTRUMENTS
Adding or Changing
• NI-DAQmx 9.5.1
NI MAX Configuration Support
Application Development Support
• NI I/O Trace 3.0
• NI Measurement & Automation Explorer 5.1
• NI Network Browser 5.0.0
Click the Next button to begin installation. Click the Back button to change the installation settings.
Save File...
<< Back
Next >>
Cancel



7. When the message indicating that the installation has successfully completed, click the Next button and Restart the computer as instructed.


NI-DAQmx 9.5.1
Installation Complete
NATIONAL INSTRUMENTS
The features in this installation have been successfully updated. You may be prompted to reboot after dismissing this dialog.
<< Back
Next >>
Finish

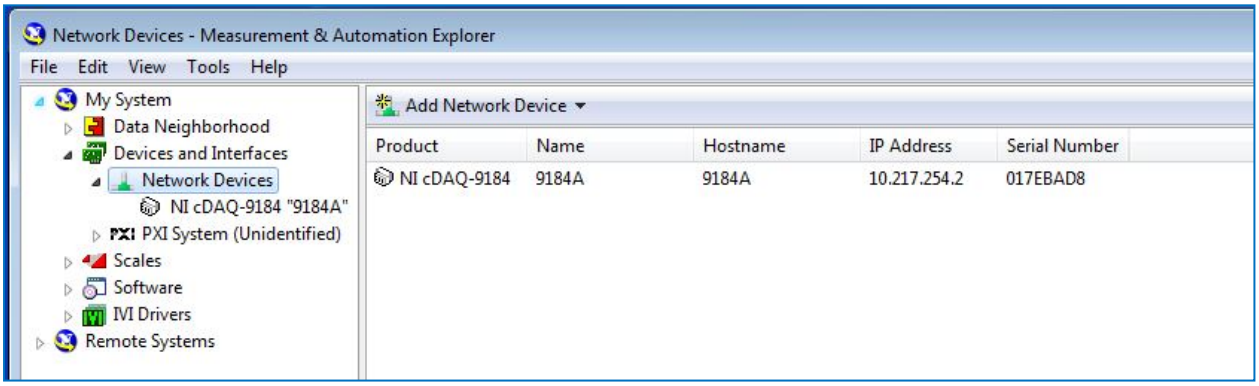

NI-DAQmx 9.5.1
You must restart your computer to complete this operation.
If you need to install hardware now, shut down the computer. If you choose to restart later, restart your computer before running any of this software.
Restart
Shut Down
Restart Later

8. Once the computer reboots, NI-DAQMX icon should be visible on the desktop

Configuring the NI-9184 Ethernet Chassis Hostname and IP Address using the NI-DAQMX Software

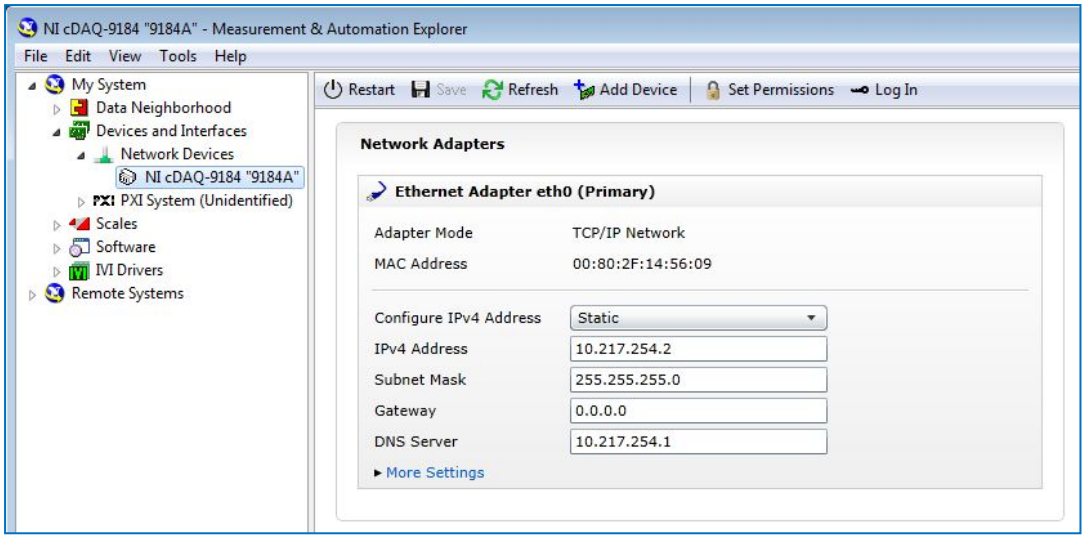
To configure a NI-9184 4-slot chassis on a CompassCDS acquisition and control client computer, the CompassCDS National Instruments control drivers should have already been installed on this computer and the NI-9184 chassis (with the NI-9219 ADC and NI-9401 TTL I/O module installed as shown in the figure below), powered on and connected either directly to the computer via an Ethernet crossover cable or indirectly via an Ethernet switch or router.

The previously installed NI-DAQMX software can then be launched from the Windows desktop and *Devices and Interfaces* selected by clicking on this option. Select the *Network Devices* option by clicking on it as shown below.



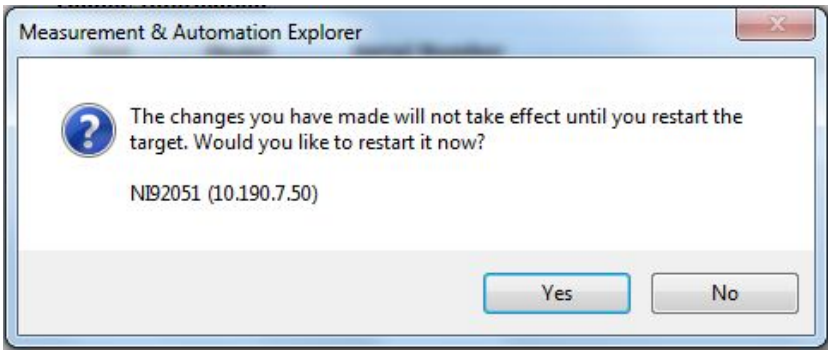
A list of the available NI-9184 chassis similar to the one shown above will appear. Clicking on the network device in the list will bring up the default Hostname and IP address as shown below. The System state will appear as *Disconnected* and the NI-9184 unit will be *Unavailable*.

Very Important: To modify the chassis Hostname, IP address, Subnet Mask and Gateway, it may be necessary to temporarily change the host computer IP and Subnet Mask to a range that matches that shown initially by the NI-9184 chassis. Once this has been done, close the NI-DAQMX software and re-open it, select *Devices and Interfaces* then *Network Devices* and click on the *NI-cDAQ-9184* module shown under Network Devices. Select the Network devices tab and editable Network Adapter fields (shown below) will be visible. The IPV4 Address should be configured as Static. Insert the IP address to be used for this device to be able to communicate with the CompassCDS acquisition client, the associated Subnet Mask, and if required, Gateway and DNS server address. Click the *Save* Icon.

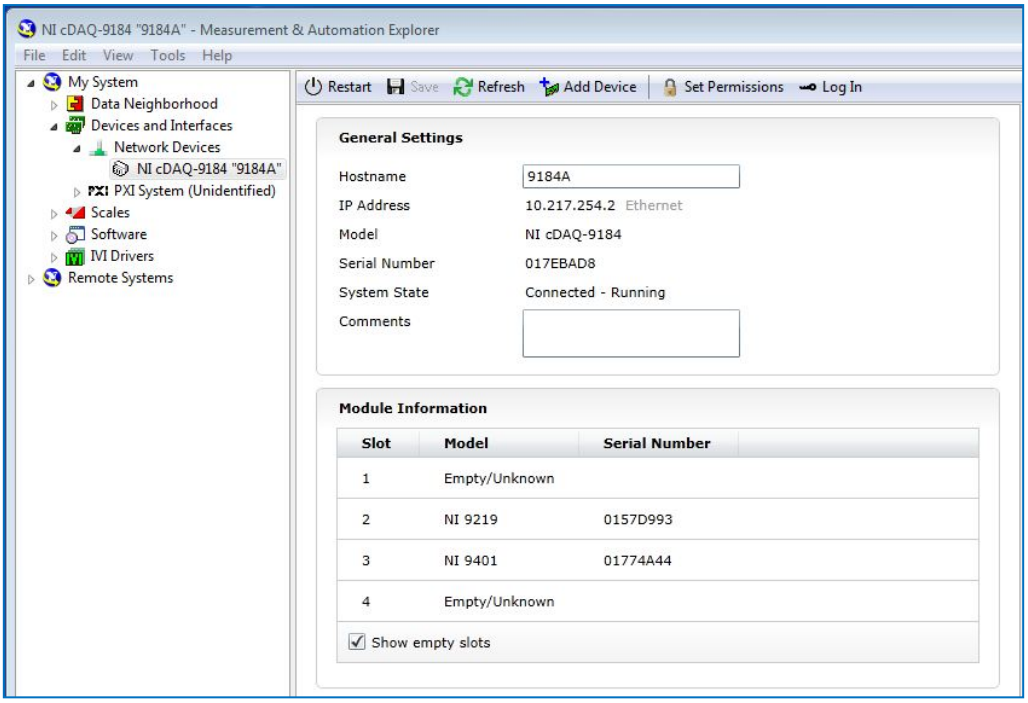


Select the General Settings tab and enter a unique Hostname. This Hostname will be required when configuring the 9184 chassis as part of a system in CompassCDS configuration manager. The new IP, Subnet Mask and Gateway addresses should be visible. Click the *Save* icon.

The following message will appear. Select Yes.

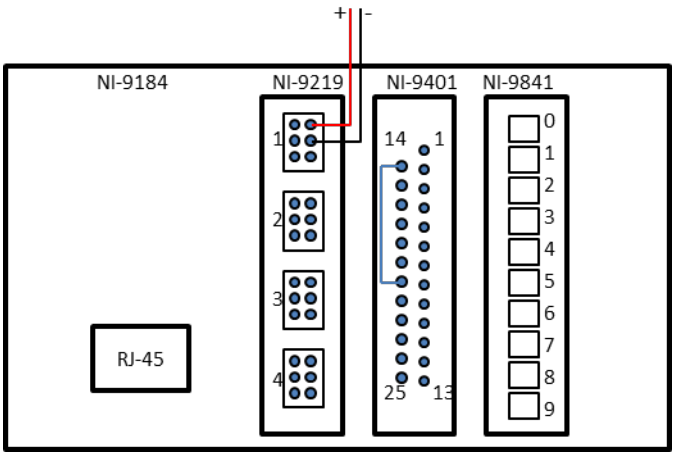

Measurement & Automation Explorer
The changes you have made will not take effect until you restart the target. Would you like to restart it now?
NI92051 (10.190.7.50)
Yes
No

Very Important: **It will now be necessary to modify the IP address and Subnet mask of the host computer back to the original settings being used for CompassCDS.** Once this has been done, re-launch the cDAQMX software and select Devices and Interfaces, Network Devices and the following screen with the modified Hostname and IP should appear and the System State should be *Running*. The installed 9219 A/D, 9401 TTL I/O and, if installed, the 9481 Relay module, should be listed (as shown below). This indicates a correctly configured NI-9184 chassis and this module can now be used to make up part of system in CompassCDS Configuration Manager.

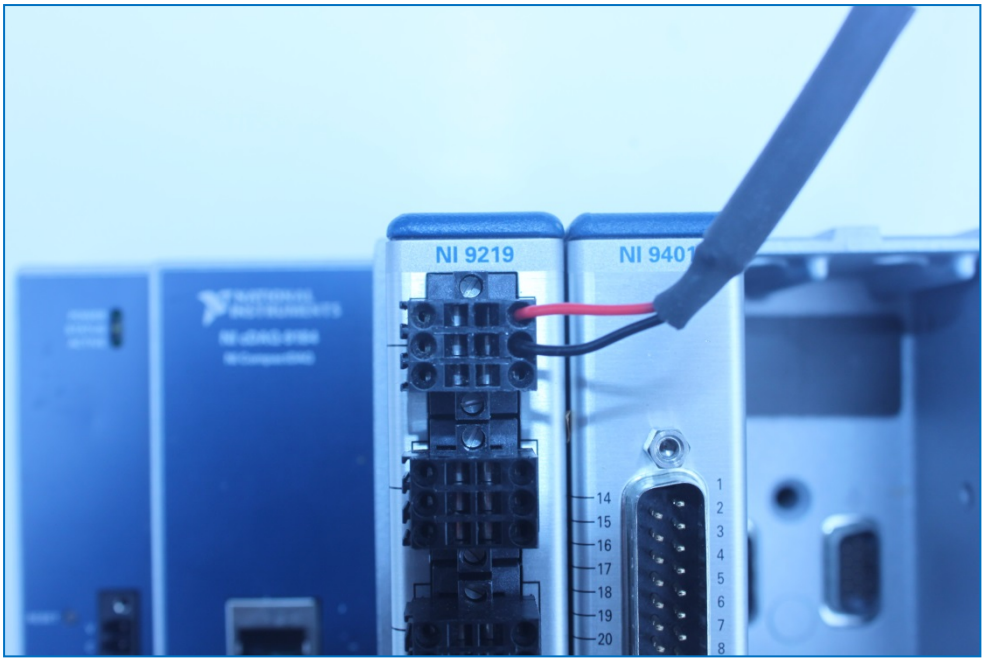

NI cDAQ-9184 "9184A" - Measurement & Automation Explorer
File Edit View Tools Help
My System
Data Neighborhood
Devices and Interfaces
Network Devices
NI cDAQ-9184 "9184A"
PXI System (Unidentified)
Scales
Software
IVI Drivers
Remote Systems
Restart Save Refresh Add Device Set Permissions Log In
General Settings
Hostname 9184A
IP Address 10.217.254.2 Ethernet
Model NI cDAQ-9184
Serial Number 017EBAD8
System State Connected - Running
Comments
Module Information
Slot Model Serial Number
1 Empty/Unknown
2 NI 9219 0157D993
3 NI 9401 01774A44
4 Empty/Unknown
Show empty slots

Connecting the NI-9219 ADC Module

The NI-9219 ADC module comprises 4x6 port connectors as shown in the diagram below. In order to connect a GC or LC detector analog output to Channel 1 of the NI-9129, the positive and negative outputs should be connected as shown below. If two detectors from the same instrument are to be connected, the same ports in the second connector should be used. The tinned ends of the cables are simply pushed into the ports after a small screwdriver (supplied with the NI-9219) has been inserted into the slot next to each port to open the connector.



Analog outputs from GC/LC detectors should be connected as shown below.



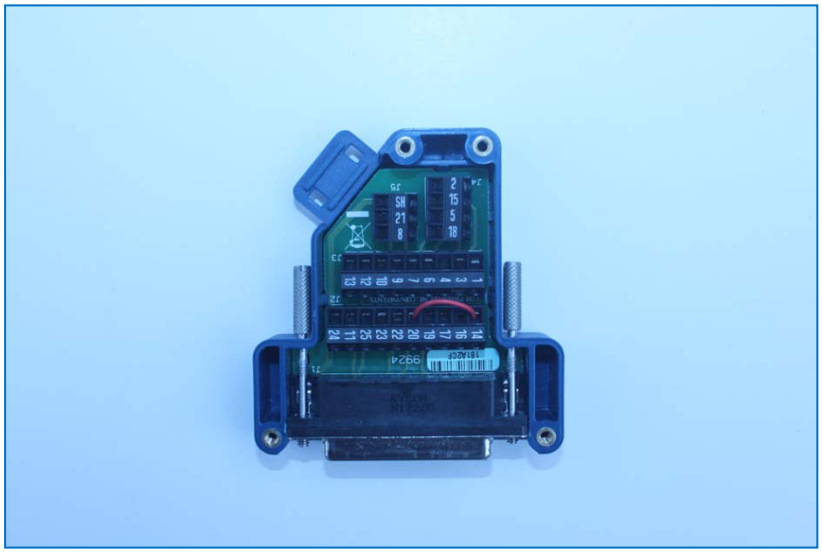
Connecting the NI-9401 TTL I/O Module as the Start In device for the NI-9219 ADC

The NI-9401 has a 25-pin DSUB connector terminal that provides connections for eight digital input/output channels. Each channel has a Digital I/O (DIO) pin to which can be connect a digital input or output device. The eight DIO channels are internally referenced to COM, so any of the nine COM lines can be used as a reference for the external signal. The DIO channels are grouped into two ports, one containing channels 0, 1, 2, and 3 (Inputs), and one containing channels 4, 5, 6, and 7 (Outputs). It is possible to independently configure each digital port for input or output however all four channels in the port must share the same line direction. Each channel also has a pull-down resistor and includes overvoltage, overcurrent, and short-circuit protection. Input and Outputs are configured as follows on the Terminal Connector.

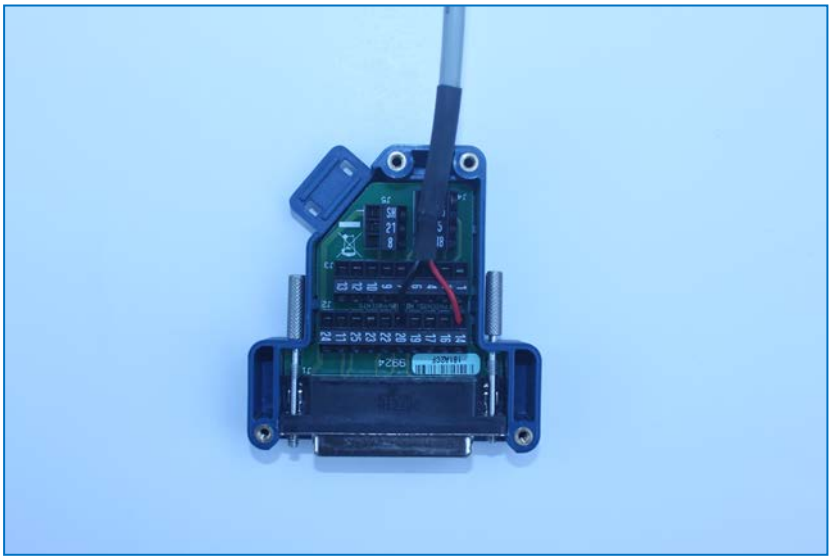
Terminals	Channel	Terminals	Channel
14 & 1	Input 1	20 & 7	Output 1
16 & 3	Input 2	22 & 9	Output 2
17 & 4	Input 3	23 & 10	Output 3
19 & 6	Input 4	25 & 12	Output 4

As the NI-9219 requires an energized start input signal (0.2-5.0 VDC) in order to initiate data acquisition, the NI-9401 module needs to be wired as follows:

1. For immediate starting of data acquisition on NI-9219 Channels 1 – 4, the NI-9401 output terminal 20 should be directly connected to input terminal 14 as shown below.

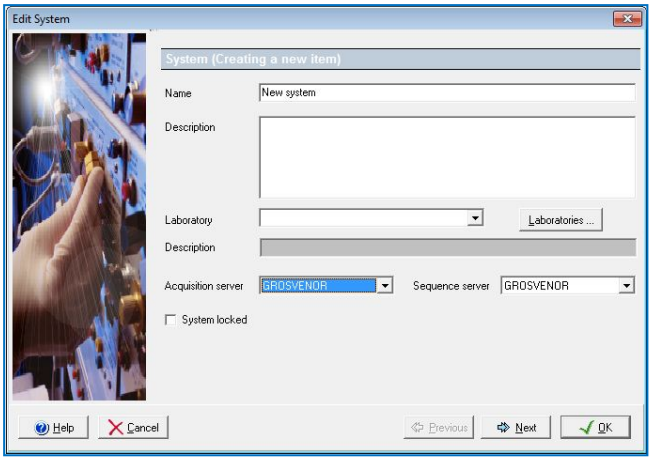


2. For starting of a system from the CompassCDS “Waiting for Injection” phase, i.e., where the start signal will come from either a contact closure or TTL device, the NI-9401 output terminal 20 and input terminal 14 should be connected as shown below.

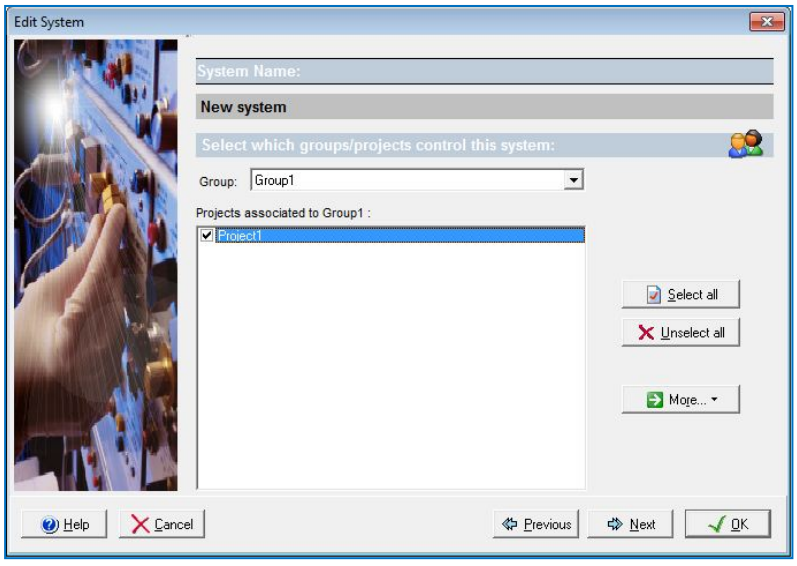


Installing the National Instruments Control Drivers and Configuring a System in Configuration Manager

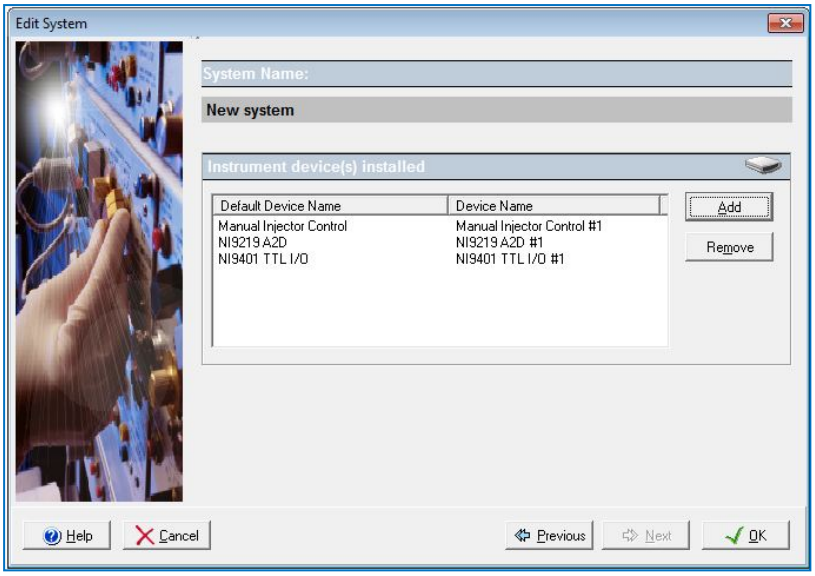
The National Instruments Control drivers for the NI-9219 module can be installed directly from the CompassCDS DVD. These drivers are located in the Drivers\SCION NI_CDAQ folder on the CompassCDS DVD. To install these drivers, run the setup.exe. Once the drivers have been installed, log into CompassCDS Configuration Manager and create a new system by selecting the Systems icon, right clicking in the Systems panel and selecting New.



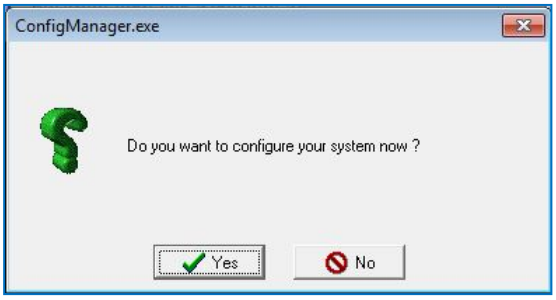
The system must be given a name (in this example New System) and have an Acquisition and a Sequence server designated as shown in the figure above. Clicking Next will bring up the Group and Project association panel. The System should be associated with at least one Group and one Project but this can also be done later via the Associations icon. Click Next to bring up the Instrument device(s) installed panel.



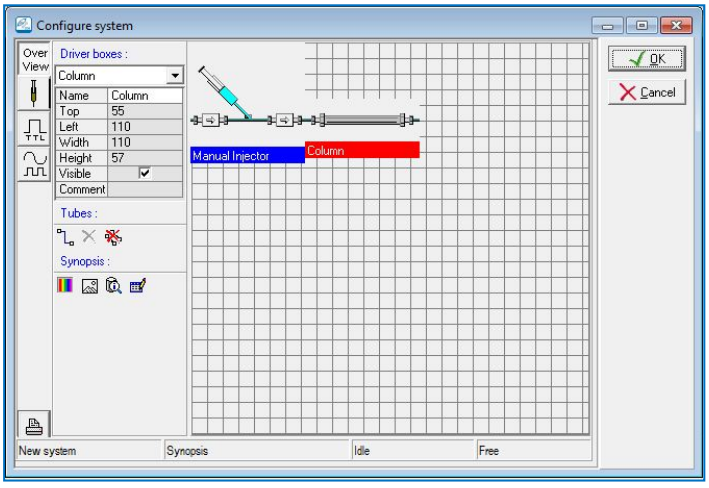
The device control drivers required for analog data acquisition with the NI-9219 module are shown in the figure below. These can be selected by clicking the Add button.



Once the three device drivers (Manual Injector, NI-9219 and NI-9401) have been selected, click the OK button and the following prompt will appear.

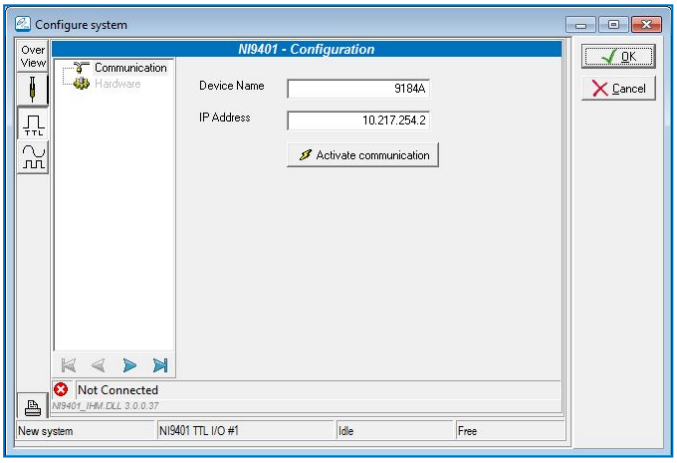


Click the Yes button and the following configuration screen (below) will appear. Select the NI-9401 by clicking on the TTL icon on the left.

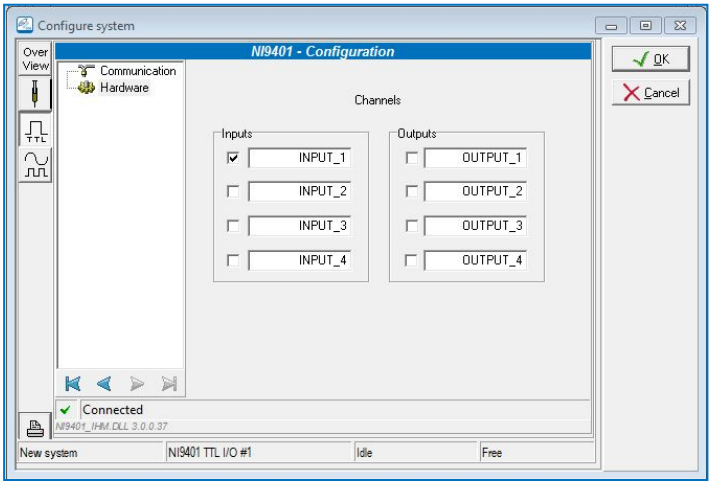


Select the Communication panel by clicking on Communication in the panel and enter the NI-9184 Chassis Hostname (originally configured by using the NI-DAQMX software) in the Device Name panel and the IP (originally configured by using the NN-DAQMX software) in the IP Address panel.

Important: Before clicking the Activate communication button, make sure the Communication (above Hardware) is highlighted in blue, by clicking on it. Now Click the Activate Communication button. Messages indicating that NI DAQ module drivers are loading will appear in the bottom right of the screen.

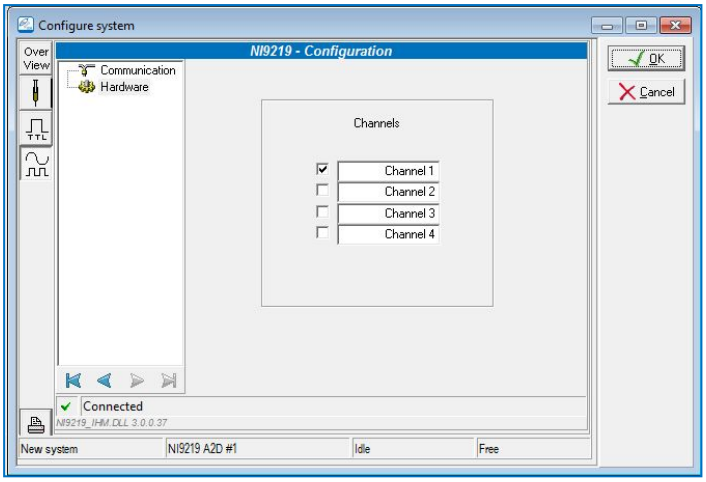


Once the drivers have completed loading, the NI-9401 Hardware option will become active and clicking on this will bring up the Input/Output Channel dialog. When the NI-9401 module is being used as the start device for the NI-9219, only the first input channel needs to be checked and all other channels must be left unchecked as shown below. The channel can be renamed if required.

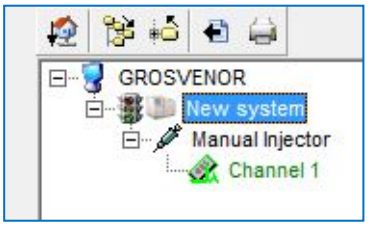


Repeat the Hostname and IP assignment procedure for the NI-9219 module.

Important: Before clicking the Activate communication button, make sure the Communication (above Hardware) is highlighted in blue, by clicking on it. When the Hardware option becomes active, Select Channel 1 as shown below and rename it if required. Click OK.

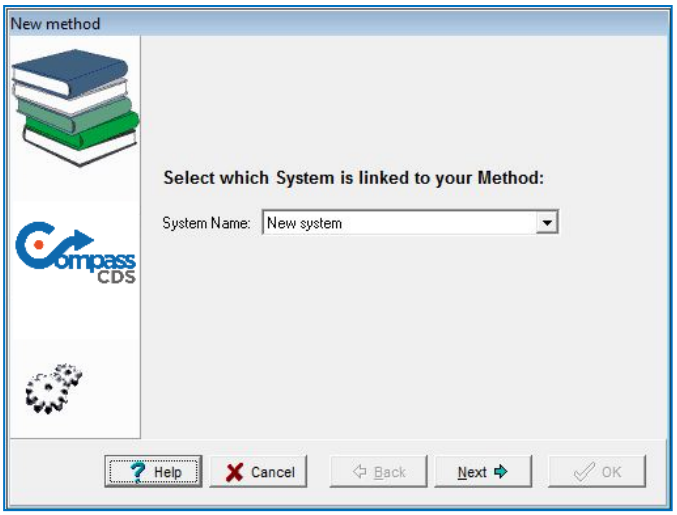


The configured system will be visible in the Stations/Systems panel in configuration manager (shown below). Select the system by clicking on the name and then right click to Stop the system. Right click again and Start the system.

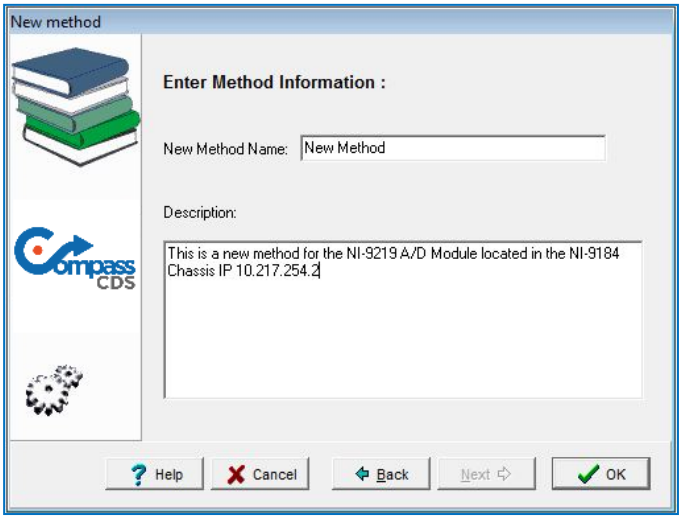


Creating a Method in CompassCDS

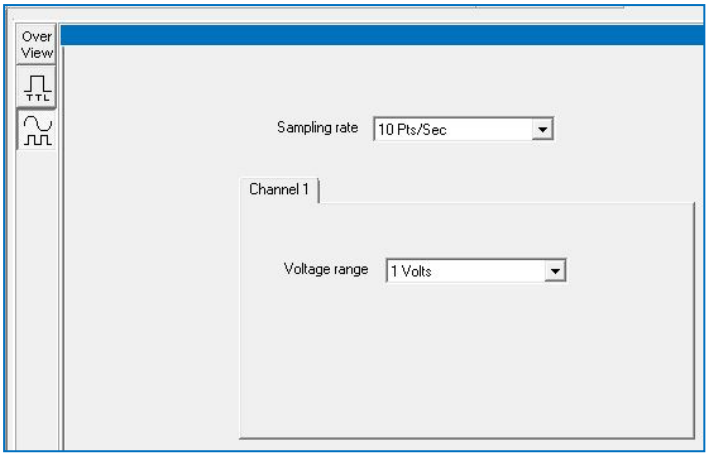
Log into CompassCDS and select File, New, New Method. The user will be prompted to select the System with which the method will be associated (in this example New system) as shown below. Click Next



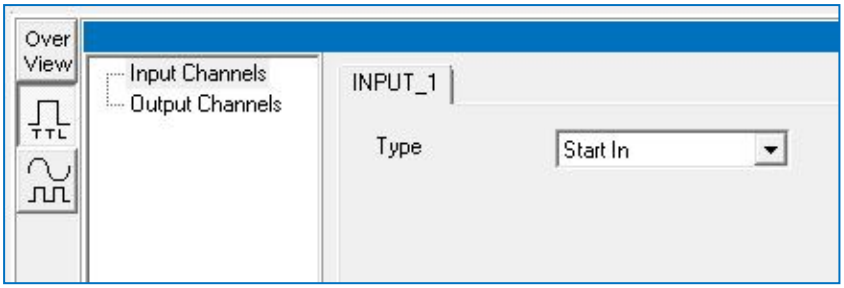
A method name and, if desired, a description of the method can be added as shown below. Clicking OK will bring up the method in the CompassCDS Data view.



Clicking on the Control section of the method tree brings up the method configuration panels for the NI-9219 and NI-9401 modules. The data sampling rate (1-100 points/second) and the voltage range (± 1, 2.5, 10V) can be selected here.



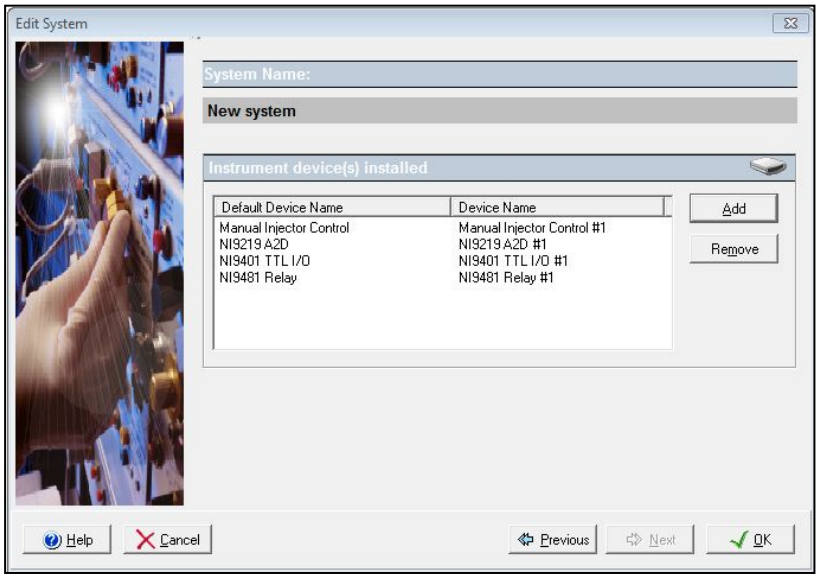
The NI-9401 module must have the input Type set to Start In as shown below.



Save and close the method once all the other relevant sections (acquisition, report style, etc.) in the method tree have been completed.

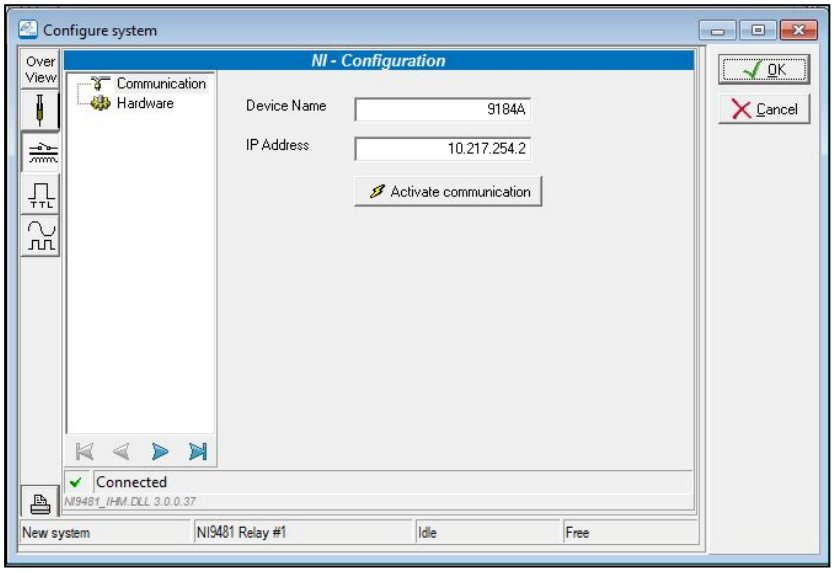
Adding the NI-9481 Relay Module as an additional module in the NI-9184 Chassis

Due to the modular nature of the NI-cDAQ devices, it is possible to add the NI-9481 contact closure relay module to the NI-9184 chassis if relay functionality is required in addition to analog data acquisition. The NI-9481 module should be inserted into the NI-9184 chassis as shown below. The NI-DAQMX software will be required to be used to assign the NI-9481 relay module a unique hostname and IP address as described previously in this guide. Once the NI-9481 module is being recognized with the correct hostname and IP address, it can be added to an existing System using Configuration Manager. The NI-9481 Relay device driver needs to be added to the system configuration as shown below.

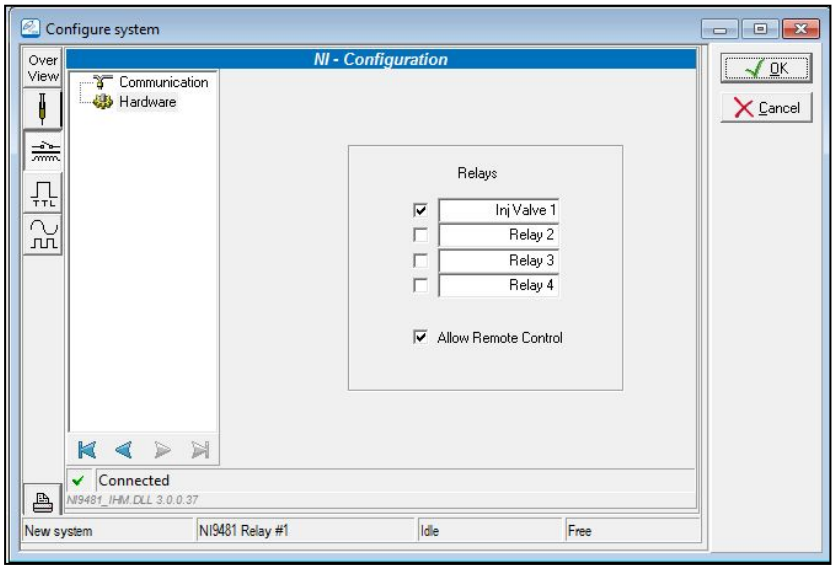


Select the Communication panel by clicking on Communication in the panel and enter the NI-9194 Chassis Hostname (originally configured by using the NI-DAQMX software) in the Device Name panel and the IP (originally configured by using the NN-DAQMX software) in the IP Address panel as shown below.

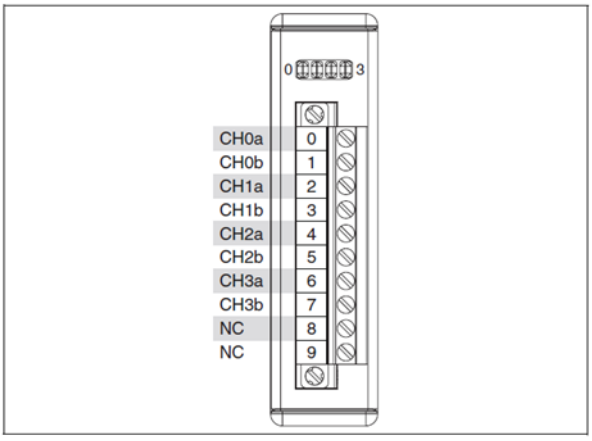
Important: **Before clicking the Activate communication button, make sure the Communication (above Hardware) is highlighted in blue, by clicking on it**. Now Click the Activate Communication button. Messages indicating that NI DAQ module drivers are loading, will appear in the bottom right of the screen.

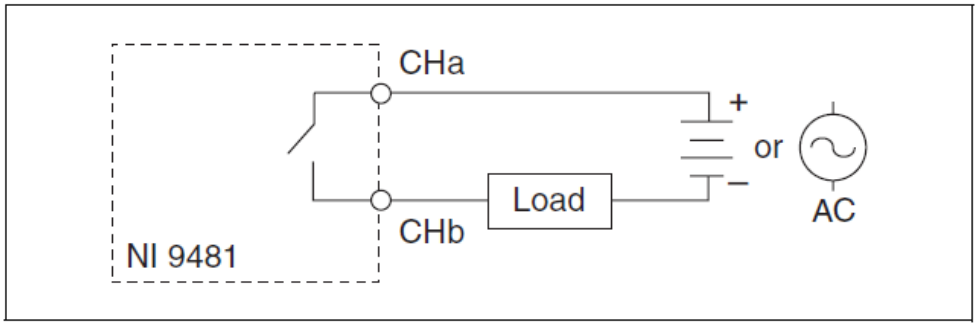


When the Hardware option becomes active, select the relay(s) to be used (see below) and also check the Allow Remote Control option if manual control of the relays from the CompassCDS system status screen is required. Click OK and stop and start the system as before.



When connecting a load to the NI-9481, connect the positive lead of the load to either the CHa or the CHb terminal, and the ground of the load to one of the leads of the power supply. Connect the remaining CHa or CHb terminal to the other lead of the power supply. An example of this type of configuration is illustrated below.


0
3
CH0a
CH0b
CH1a
CH1b
CH2a
CH2b
CH3a
CH3b
NC
NC
0
1
2
3
4
5
6
7
8
9


CHa
CHb
NI 9481
Load
+
–
or
AC

NI Modules - Technical Specifications

NI-9184 Chassis

Power Requirements	15 W
Number of Chassis Slots	4
Total Available Power	15 W
Input Voltage Range	9 V - 30 V
Built-In Trigger	No
A/D Resolution	32 bits
Network protocols	TCP/IP, UDP
Network ports used	HTTP:80 (configuration only),
	TCP:3580;
	UDP:5353 (configuration only),
	TCP:5353 (configuration only);
	TCP:31415;
	UDP:7865 (configuration only),
	UDP:8473 (configuration only)
Network IP configuration	DHCP + Link-Local, DHCP, Static, Link-Local Network interface
NI cDAQ-9184	100 Base-TX, full-duplex
	100 Base-TX, half-duplex
	10 Base-T, full-duplex
	10 Base-T, half-duple
Communication rates	
NI cDAQ-9184	10/100 Mbps, auto-negotiated
Maximum cabling distance	100 m/segment
Voltage input range	9 to 30 V
Weight (unloaded)	Approx. 470 g (16.6 oz)
Dimensions (unloaded)	194.0 × 88.7 × 33.6 mm (7.64 × 3.49 × 1.32 in.)
Operating Temperature (IEC-60068-2-1 and IEC-60068-2-2)	
NI cDAQ-9184.	0 to 55 °C
Ingress protection	IP 30
Operating Humidity (IEC-60068-2-56)	10 to 90% RH, noncondensing

This module meets the requirements of the following standards of safety for electrical equipment for measurement, control, and laboratory use: IEC 61010-1, EN 61010-1, UL 61010-1, CSA 61010-1

NI-9219 ADC Module

Differential Input Channels	4
Resolution	24 bits
Sample Rate	100 pts/s
Maximum Voltage Range	-60 V - 60 V
Minimum Voltage Range	-0.125 V - 0.125 V
Excitation Voltage	2.5 V
Length	9 cm
Width	2.3 cm

NI-9401 TTL I/O Module

Number of channels	8 DIO channels
Default power-on line direction	Input
Input/output type	TTL, single-ended
Input Voltage	5.25 V max
High, VIH	2 V min
Low, VIL	0.8 V max
Output	
Output Voltage High, VOH	5.25 V max
Output Voltage Low	
Sinking 100 µA	0.1 V max
Sinking 2 mA	0.4 V max
Operating temperature (IEC 60068-2-1, IEC 60068-2-2)	–40 to 70 °C
Operating humidity (IEC 60068-2-56)	10 to 90% RH, noncondensing

Safety Standards **-** This module is designed to meet the requirements of the following standards of safety for electrical equipment for measurement, control, and laboratory use: IEC 61010-1, EN 61010-1, UL 61010-1, CSA 61010-1

CompassCDS
National Instruments NI-9481 Relay & NI-9401 TTL I/O Module User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501616
Revision A

Contents

Introduction 3
NI-DAQmx Software Installation 4
NI-9181 Ethernet Chassis Configuration 7
Connecting the NI-9481 Relay Module 10
Configuring the NI-9481 Relay Module in CompassCDS 11
Connecting the NI-9401 TTL I/O Module 12
Configuring the NI-9401 TTL I/O Module 13
NI Hardware Technical Specifications 15
- NI-9481 Relay Module 18
  - Output Characteristics 18
  - Power Requirements 18
  - Safety Voltages 19
  - Hazardous Locations 19
  - Safety Standards 19
  - Electromagnetic Compatibility 19
  - CE Compliance 19
- NI-9401 TTL I/O Module 20
  - Input/Output Characteristics 20
  - Digital logic levels 20
  - Safety Standards 21
  - Hazardous Locations 21
  - Environmental 21
  - CE Compliance 22

Introduction

The National Instruments NI-9181 single slot chassis can be used in conjunction with the NI-9481 Relay module or the NI-9401 TTL I/O module to facilitate triggering of external devices and instruments such as valves and autosamplers etc. within the CompassCDS software as well as for triggering of the CompassCDS software by external devices.

The standard 4 channel relay interface module configuration for CompassCDS (part number BR502096) includes the NI-9181 single-slot Ethernet chassis and power supply as well as the 4 Channel, 30-60VDC, 250 VAC NI-9481 Relay Module and terminal connector kit shown below.

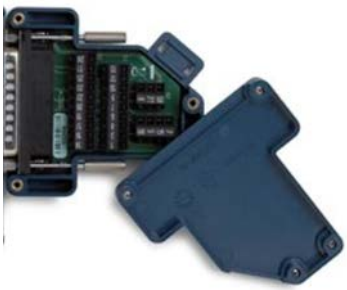
NI-9181

NI-9481

The standard TTL I/O interface module configuration for CompassCDS (part number BR502098) includes the NI-9181 single-slot Ethernet chassis and power supply as well as a NI-9401 8 Channel TTL Digital Input/Output module and terminal connector kit shown below.

NI-9181

NI-9401 TTL I/O

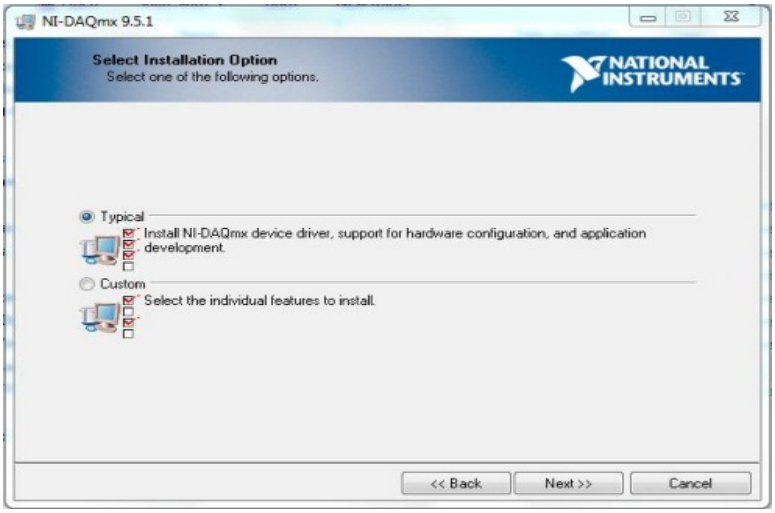


NI-9924

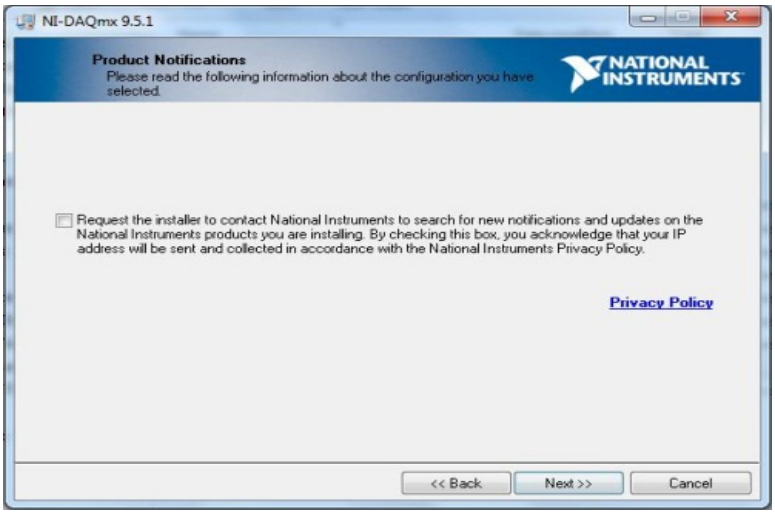
NI-DAQmx Software Installation

The National Instruments NI-DAQmx software is required to be installed in order to a) configure the NI-9181 Chassis and b) operate the NI-9481 Relay and NI-9401 TTL I/O modules. This software is supplied on a CD with the NI-9181 Chassis and can also be downloaded from the National Instruments website www.nationalinstruments.com

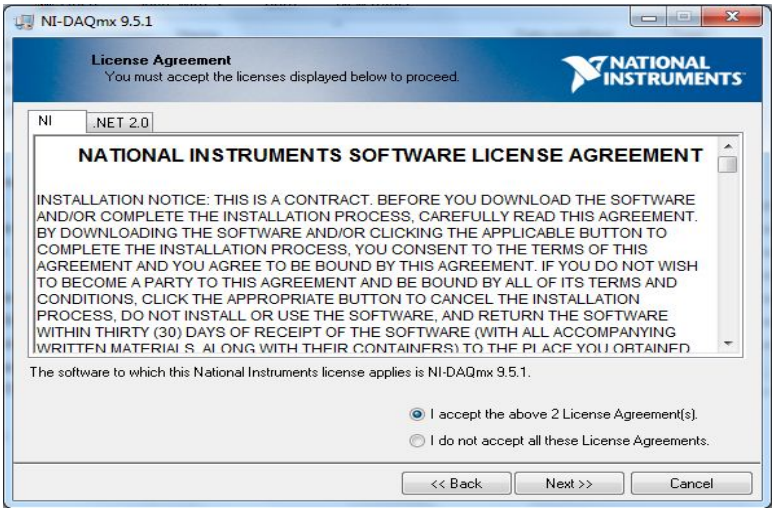
Insert the CD into appropriate drive on the computer and the autorun will prompt the installer to select either a Typical or Custom installation. The Typical installation option should be selected and Next clicked.



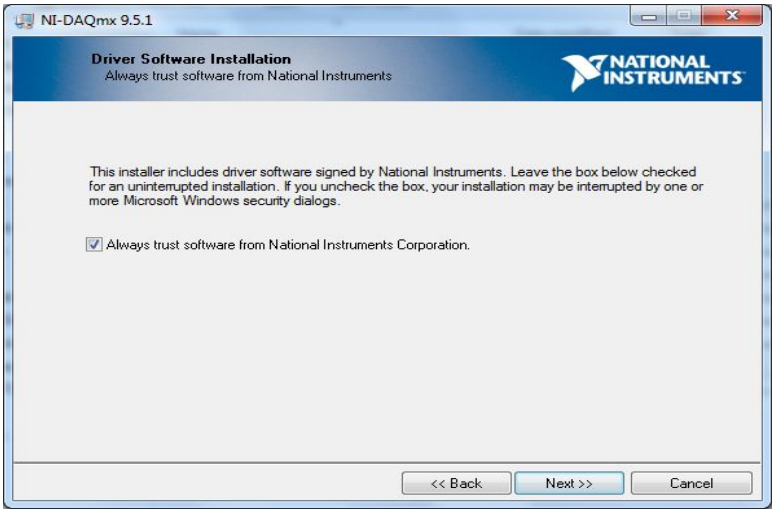
Do not check the “Request the installer to contact National Instruments”…. Box, simply click Next


NI-DAQmx 9.5.1
Product Notifications
Please read the following information about the configuration you have selected.
NATIONAL INSTRUMENTS
Request the installer to contact National Instruments to search for new notifications and updates on the National Instruments products you are installing. By checking this box, you acknowledge that your IP address will be sent and collected in accordance with the National Instruments Privacy Policy.
Privacy Policy
<< Back
Next >>
Cancel

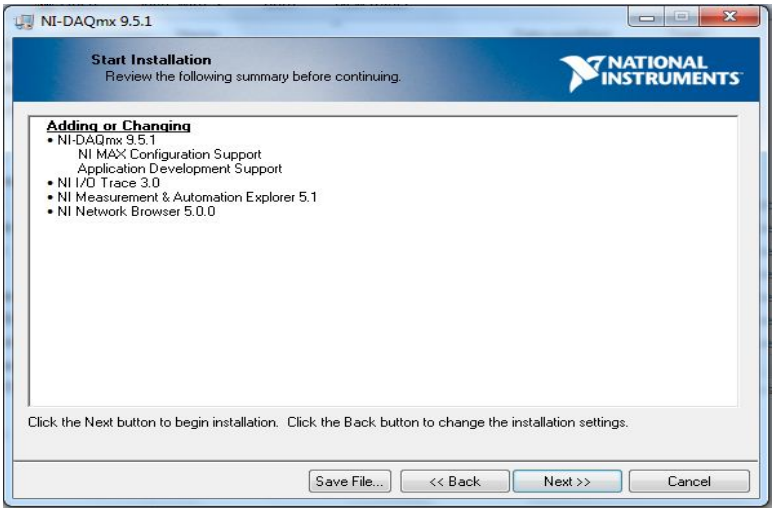
The installer should read the National Instruments software license agreement and then accept the 2 licenses by checking the radio button before clicking the Next option as shown below.


NI-DAQmx 9.5.1
License Agreement
You must accept the licenses displayed below to proceed.
NATIONAL INSTRUMENTS
NI
.NET 2.0
NATIONAL INSTRUMENTS SOFTWARE LICENSE AGREEMENT
INSTALLATION NOTICE: THIS IS A CONTRACT. BEFORE YOU DOWNLOAD THE SOFTWARE AND/OR COMPLETE THE INSTALLATION PROCESS, CAREFULLY READ THIS AGREEMENT. BY DOWNLOADING THE SOFTWARE AND/OR CLICKING THE APPLICABLE BUTTON TO COMPLETE THE INSTALLATION PROCESS, YOU CONSENT TO THE TERMS OF THIS AGREEMENT AND YOU AGREE TO BE BOUND BY THIS AGREEMENT. IF YOU DO NOT WISH TO BECOME A PARTY TO THIS AGREEMENT AND BE BOUND BY ALL OF ITS TERMS AND CONDITIONS, CLICK THE APPROPRIATE BUTTON TO CANCEL THE INSTALLATION PROCESS, DO NOT INSTALL OR USE THE SOFTWARE, AND RETURN THE SOFTWARE WITHIN THIRTY (30) DAYS OF RECEIPT OF THE SOFTWARE (WITH ALL ACCOMPANYING WRITTEN MATERIALS, ALONG WITH THEIR CONTAINERS) TO THE PLACE YOU OBTAINED
The software to which this National Instruments license applies is NI-DAQmx 9.5.1.
I accept the above 2 License Agreement(s).
I do not accept all these License Agreements.
<< Back
Next >>
Cancel

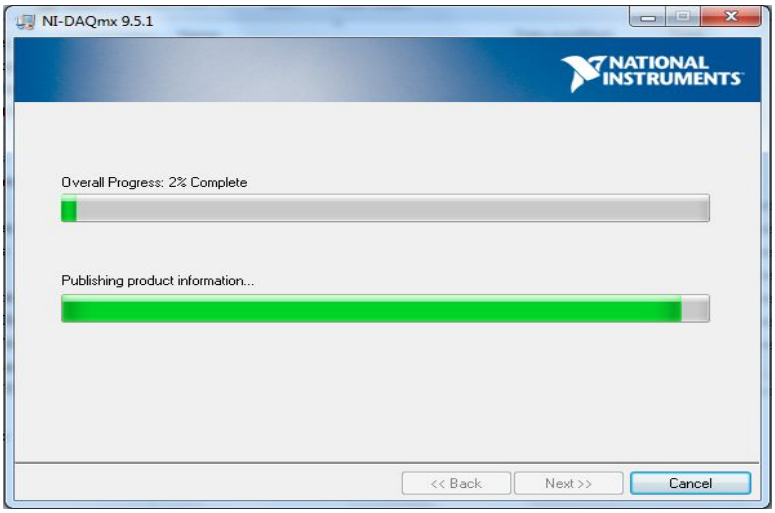
The installer should then check the “Always trust software from National Instruments Corporation checkbox and click the Next option as shown below.


NI-DAQmx 9.5.1
Driver Software Installation
Always trust software from National Instruments
NATIONAL INSTRUMENTS
This installer includes driver software signed by National Instruments. Leave the box below checked for an uninterrupted installation. If you uncheck the box, your installation may be interrupted by one or more Microsoft Windows security dialogs.
Always trust software from National Instruments Corporation.
<< Back
Next >>
Cancel

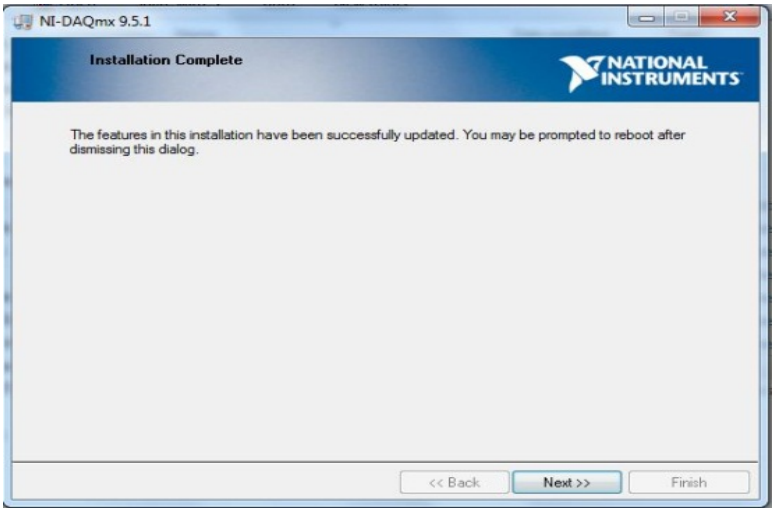
The installer should then click the Next button (see below) to start the installation of the NI-DAQmx software


NI-DAQmx 9.5.1
Start Installation
Review the following summary before continuing.
NATIONAL INSTRUMENTS
Adding or Changing
• NI-DAQmx 9.5.1
NI MAX Configuration Support
Application Development Support
• NI I/O Trace 3.0
• NI Measurement & Automation Explorer 5.1
• NI Network Browser 5.0.0
Click the Next button to begin installation. Click the Back button to change the installation settings.
Save File...
<< Back
Next >>
Cancel

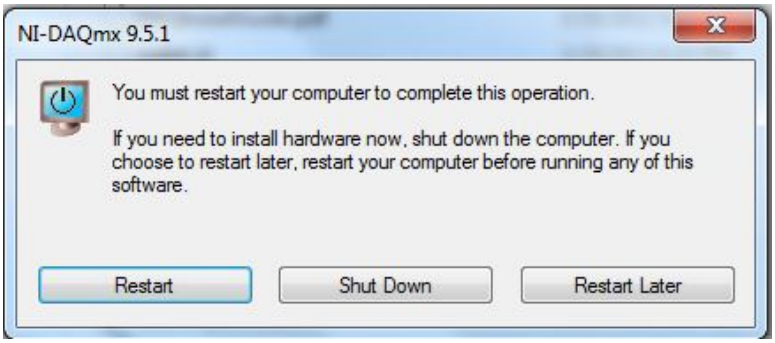
The NI-DAQmx software installation process can take some time and can be monitored by observing the Overall Progress bar as shown below.



When the installation completes, the installer will be prompted to reboot the computer and he/she should click the Next option.


NI-DAQmx 9.5.1
Installation Complete
NATIONAL INSTRUMENTS
The features in this installation have been successfully updated. You may be prompted to reboot after dismissing this dialog.
<< Back
Next >>
Finish

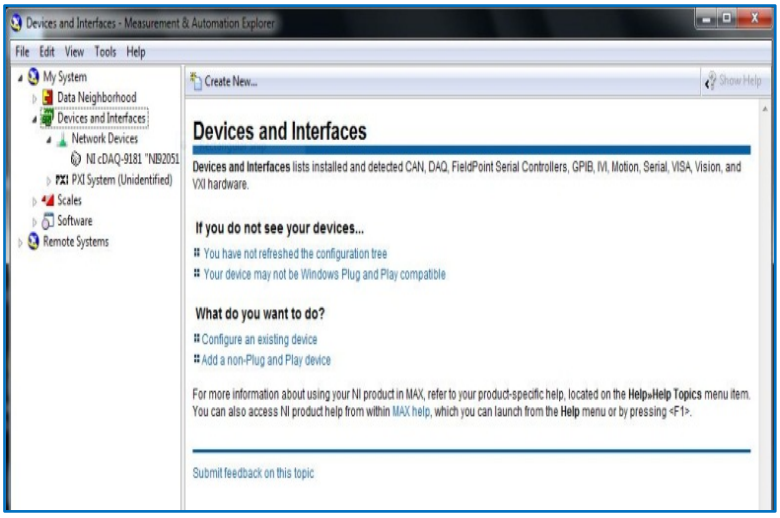
Click the Restart option and allow the computer to reboot.


NI-DAQmx 9.5.1
You must restart your computer to complete this operation.
If you need to install hardware now, shut down the computer. If you choose to restart later, restart your computer before running any of this software.
Restart
Shut Down
Restart Later

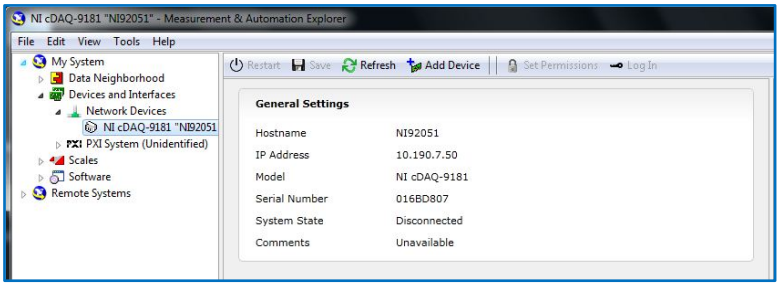
The NI-DAQmx software is now installed and can be used to configure the NI-9181 single-slot chassis and associated NI-9481 and NI-9401 modules as described below.

NI-9181 Ethernet Chassis Configuration

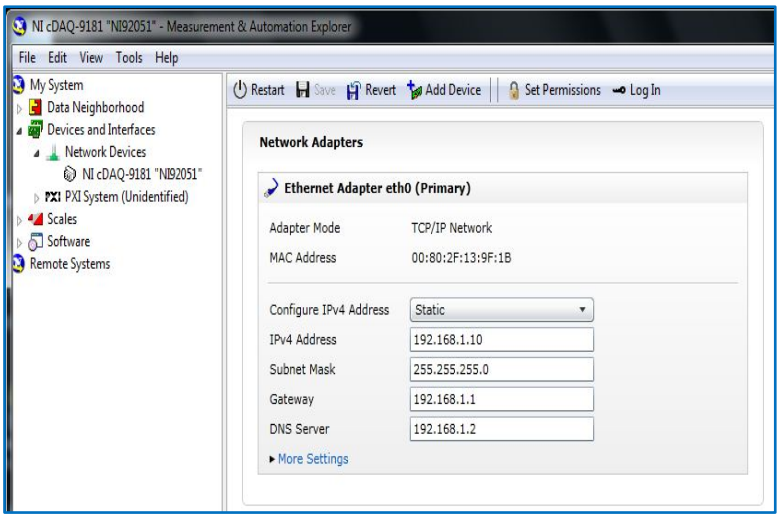
Before the NI-9181 single-slot chassis can be used with the CompassCDS software, it has to be assigned a unique name and a static IP address. The NI-9181 should be powered on and connected directly to the computer via an Ethernet crossover cable or indirectly via an Ethernet switch. The user launches the NI-DAQmx software from the desktop icon ( ) and selects the Devices and Interfaces, followed by the Network Devices option. The NI-9181 module should listed under Network Devices as shown below.


Devices and Interfaces - Measurement & Automation Explorer
File Edit View Tools Help
My System
Data Neighborhood
Devices and Interfaces
Network Devices
NI cDAQ-9181 "NI92051"
PXI System (Unidentified)
Scales
Software
Remote Systems
Create New...
Show Help
Devices and Interfaces
Devices and Interfaces lists installed and detected CAN, DAQ, FieldPoint Serial Controllers, GPIB, IVI, Motion, Serial, VISA, Vision, and VXI hardware.
If you do not see your devices...
You have not refreshed the configuration tree
Your device may not be Windows Plug and Play compatible
What do you want to do?
Configure an existing device
Add a non-Plug and Play device
For more information about using your NI product in MAX, refer to your product-specific help, located on the Help»Help Topics menu item. You can also access NI product help from within MAX help, which you can launch from the Help menu or by pressing <F1>.
Submit feedback on this topic

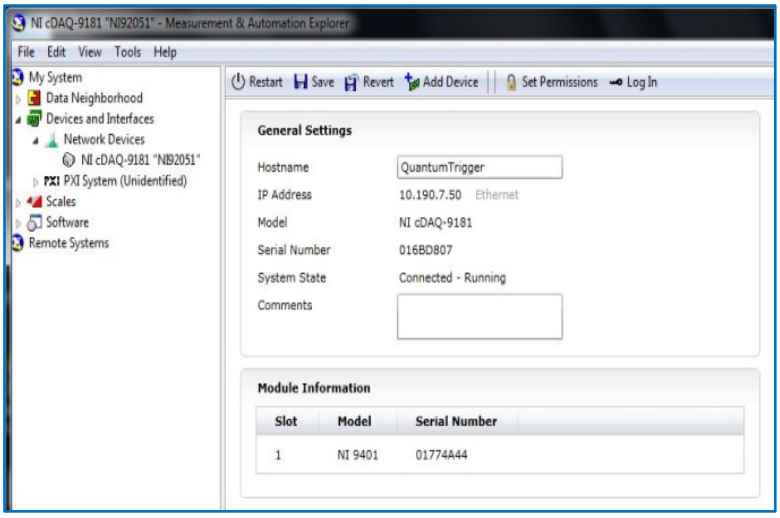
Select the NI-9181 module by clicking on it and the module settings will appear as shown below. The NI-9181 module requires a unique Hostname and IP Address



The IP Address can be changed by selecting the Settings tab. The assigned IP should be static, have a suitable Subnet Mask, Gateway IP and if required, a DNS server IP.

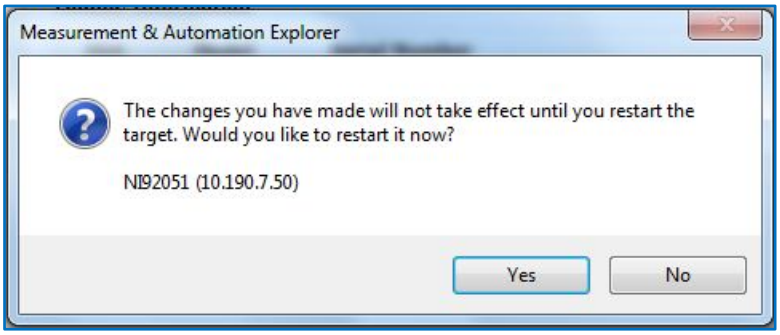


The Hostname can be changed from the General Settings tab. Once the IP and Hostname have been changed, it is necessary to click on the Save option to make these permanent.

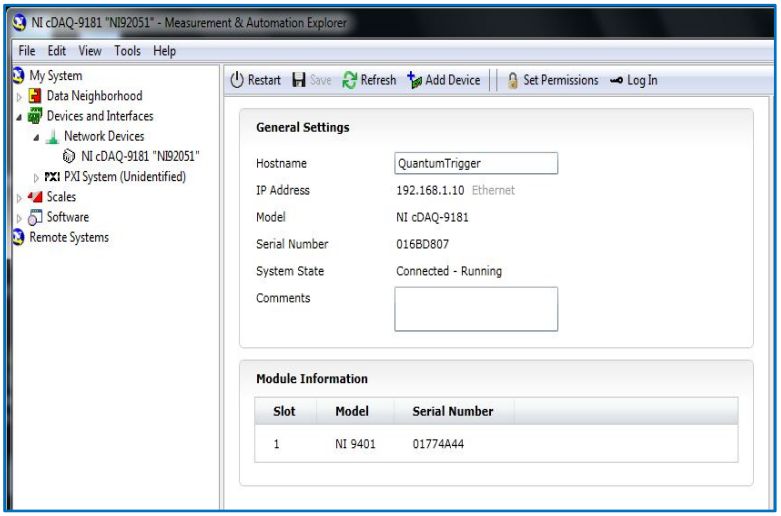


Restart the NI-9181 Chassis by clicking on the Restart option or by selecting the Yes option as shown below.

Note: the NI-9481 Relay or NI-9401 TTL I/O modules can be inserted into the NI-9181 module before the restart. The NI-9181 should be powered down before either of these modules is inserted.

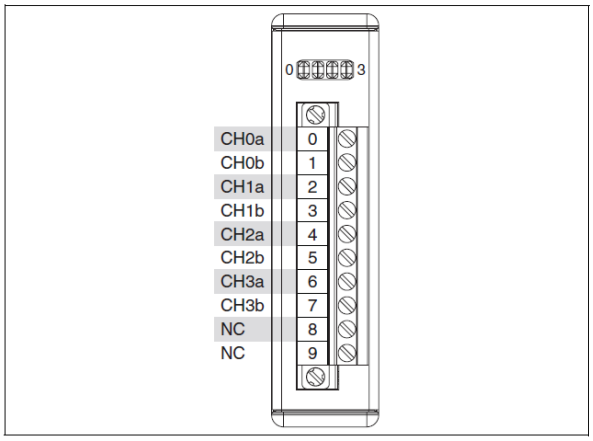

Measurement & Automation Explorer
The changes you have made will not take effect until you restart the target. Would you like to restart it now?
NI92051 (10.190.7.50)
Yes
No

Selecting the configured NI-9181 under Network Devices should display the new device Hostname and IP address. The inserted NI module (9481 or 9401) and its associated serial number should also now be visible in the Module Information section as shown below.

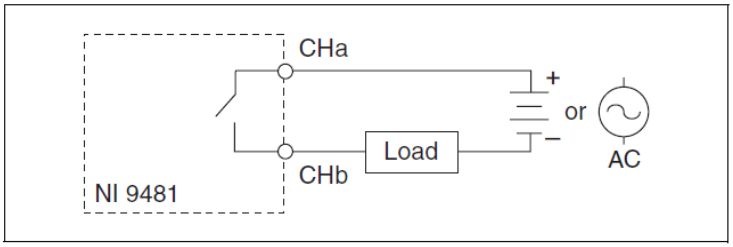


Connecting the NI-9481 Relay Module

The NI-9481 has a 10-terminal detachable screw-terminal connector that provides connections for 4 electromechanical relay channels. Each electromechanical relay channel has two interchangeable terminals, CHa and CHb. Each channel has an LED that indicates the state of the channel. When a channel LED is lit, the channel is on i.e. the relay is closed. When the LED is un-lit, the channel is off and the relay is open. Relay 1 is represented by CH0a and CH0b, i.e. screw terminals 0 & 1 as shown in the diagram below. Relay 2 is represented by CH1a and CH1b, i.e. screw terminals 2 & 3.



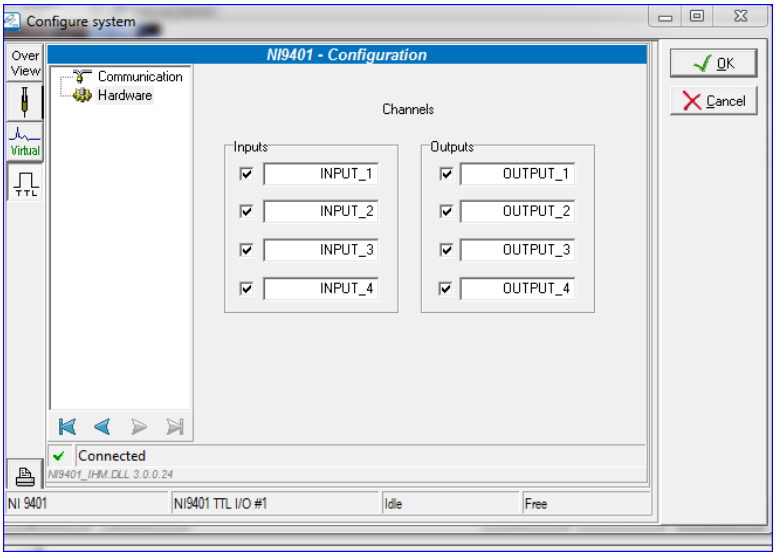
When connecting a load to the NI-9481, the positive lead of the load should be connected to either the CHa or the CHb terminal, and the ground of the load to one of the leads of the power supply. Connect the remaining CHa or CHb terminal to the other lead of the power supply. An example of this type of configuration is illustrated below.



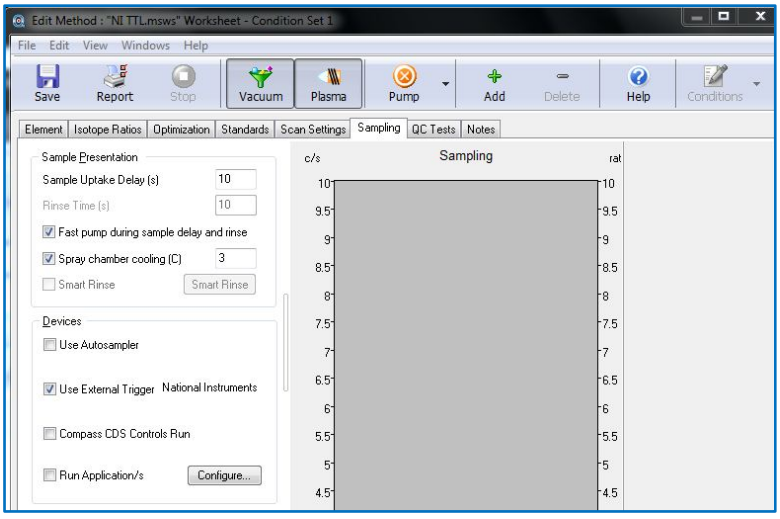
Configuring the NI-9481 Relay Module in CompassCDS

The NI-9481 Relay module is configured from within the CompassCDS Configuration Manager. The relay module is usually added as part of an existing GC or LC system. Users select Systems, New, name the system and select the appropriate acquisition and sequence server from the dropdown list and click Next. A Group and Project(s) is selected and Next is clicked. The empty instrument device(s) installed dialog window appears and the user selects the 9181 and the 9481 control drivers as well as any other drivers required to build a GC or LC system before clicking Next.

The NI-9181 module IP address should be entered in the Address box and the Activate Communication button clicked. The Hostname will appear along with the 9481 graphical user interface (GUI) below the hostname. The Device Status should indicate *Connected***.** The relay timetable can be used to set up complex relay triggering if required.

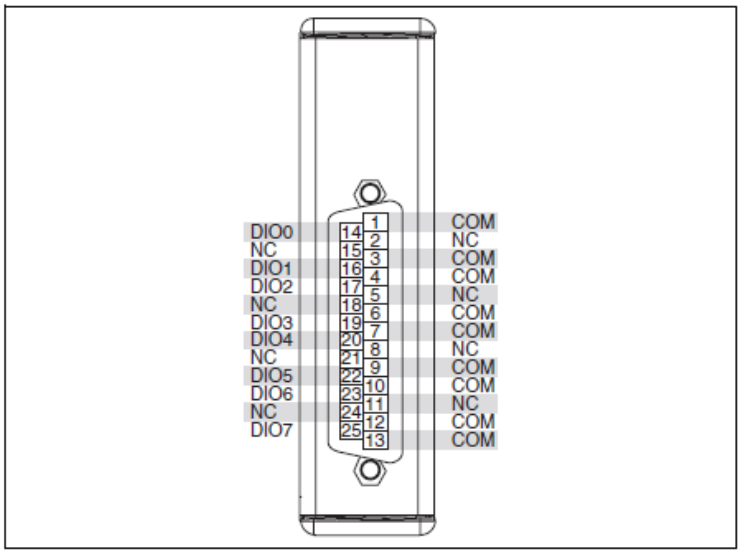


Once the relay device has been set up in Config Manager, the only additional setting is located within the CompassCDS method where the user must check the Use External Trigger checkbox as shown below. Once the method is saved, external triggering of the relay will be active.

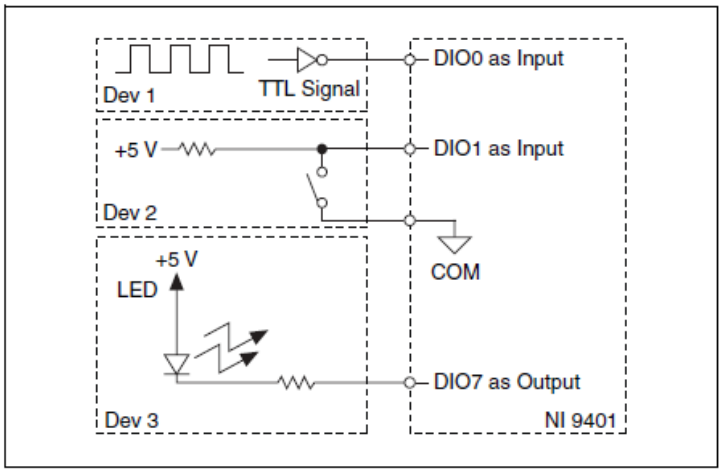


Connecting the NI-9401 TTL I/O Module

The NI 9401 has a 25-pin DSUB connector that provides connections for eight digital input/output channels. Each channel has a Digital I/O (DIO) pin to which you can connect a digital input or output device. The eight DIO channels are internally referenced to COM, so you can use any of the nine COM lines as a reference for the external signal. The DIO channels are grouped in two ports, one containing channels 0, 1, 2, and 3, and one containing channels 4, 5, 6, and 7. It is possible to independently configure each digital port for input or output however all four channels in the port must share the same line direction. Each channel also has a pull-down resistor and includes overvoltage, overcurrent, and short-circuit protection. DIO0 or Channel 1 = screw terminals 14 & 1 is configured as an input channel in the CompassCDS software. DIO4 or Channel 5 = screw terminals 20 & 7 is configured as an output channel (5 VDC) in the CompassCDS software.

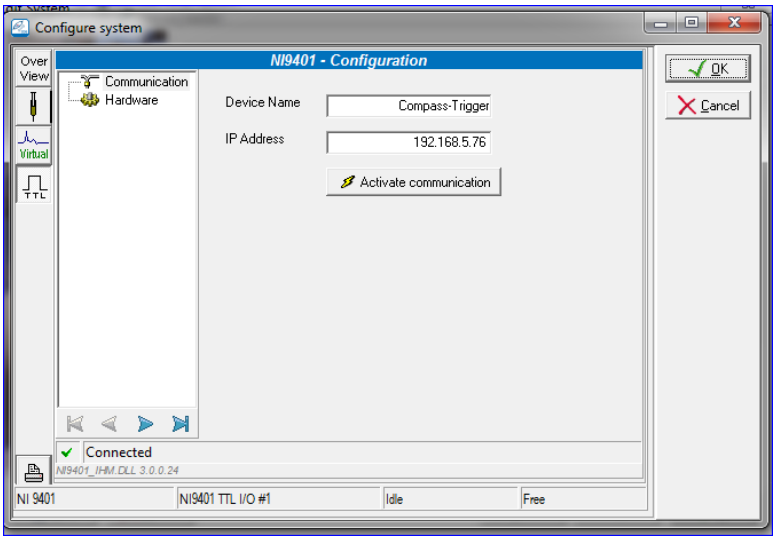


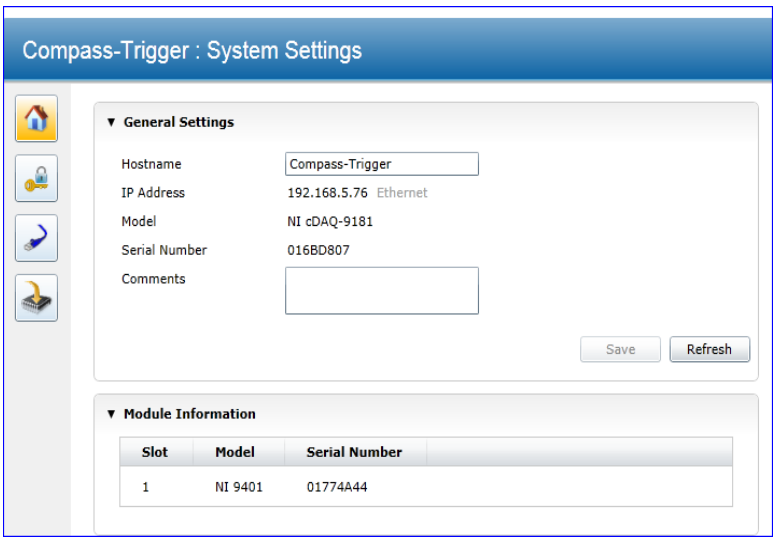
Example NI-9401 input and output connection configurations are shown below.

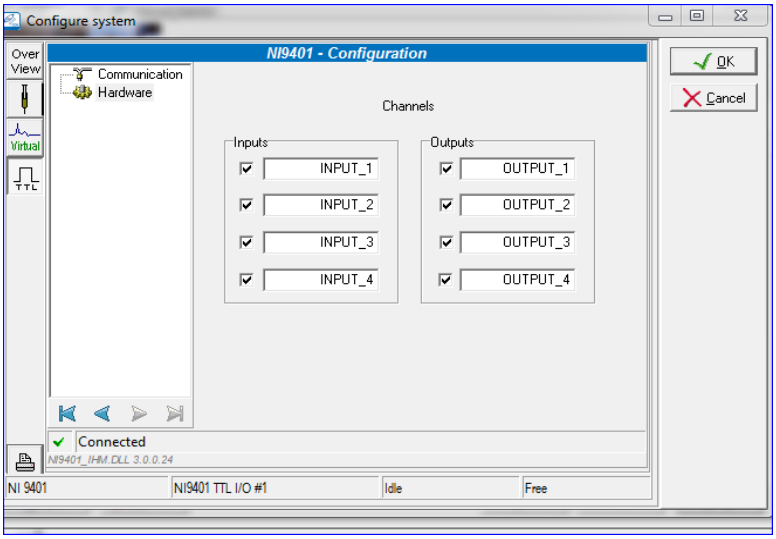


Configuring the NI-9401 TTL I/O Module

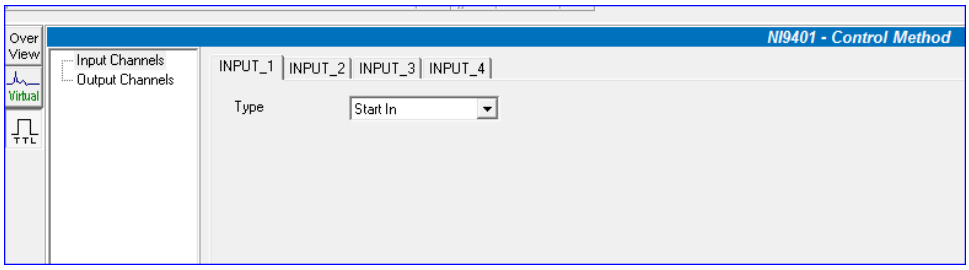
The NI-9401 TTL I/O module is configured within CompassCDS from the Config Manager. Users should click on this tab and then the Hardware field, selecting the National Instruments option from the dropdown list as shown below. The NI-9181 module IP address should be entered in the Address box and the Activate Communication button clicked. The Hostname will appear along with the 9401 graphical user interface (GUI) below the hostname. The Device Status should indicate *Connected***.** The user can now select either the Input or the Output option. The timetable can be used to set up complex I/O triggering if this is required.

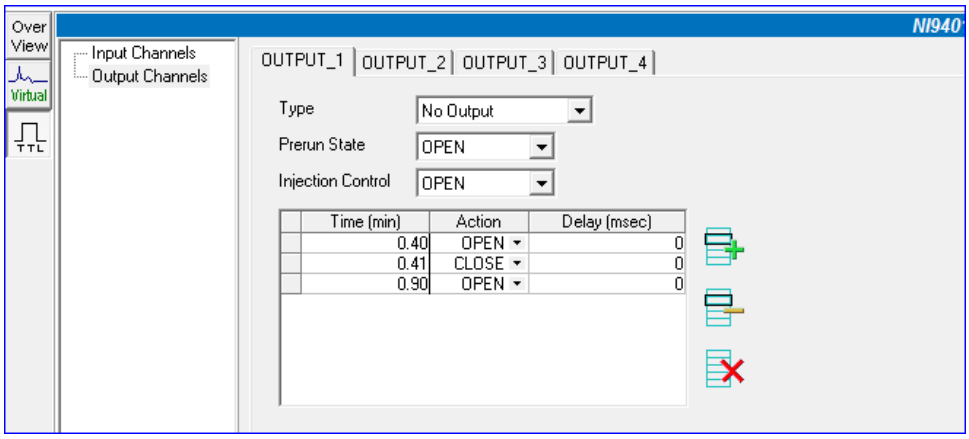






Once the TTL I/O device has been set up in Config Manager, the only additional setting is located within the CompassCDS method where the user has to select the Input or Output sections as shown below. Once the method is saved and Services are stopped and started, TTL I/O triggering will be active.





NI Hardware Technical Specifications

NI-9181 Chassis

Network Protocols	TCIP, UDP
Network ports used	HTTP:80 (configuration only) TCP:3580 UDP:5353 (configuration only) TCP:5353 (configuration only) TCP:31415 UDP:7865 (configuration only) UDP:8473 (configuration only)
Network IP configuration	DHCP + Link-Local, DHCP, Static, Link-Local
Network interface	
NI cDAQ-9181	100 Base-TX, full-duplex 100 Base-TX, half-duplex 10 Base-T, full-duplex 10 Base-T, half-duplex
Communication rates	
NI cDAQ-9181	10/100 Mbps, auto-negotiated
Maximum cabling distance	100 m/segment

Input/output voltage protection

Voltage	Minimum	Maximum
Input	–20 V	25 V
Output	–15 V	20 V

Maximum operating conditions[1]

Level	Minimum	Maximum
I_{OL} output low current	—	8 mA
I_{OH} output high current	—	–8 mA

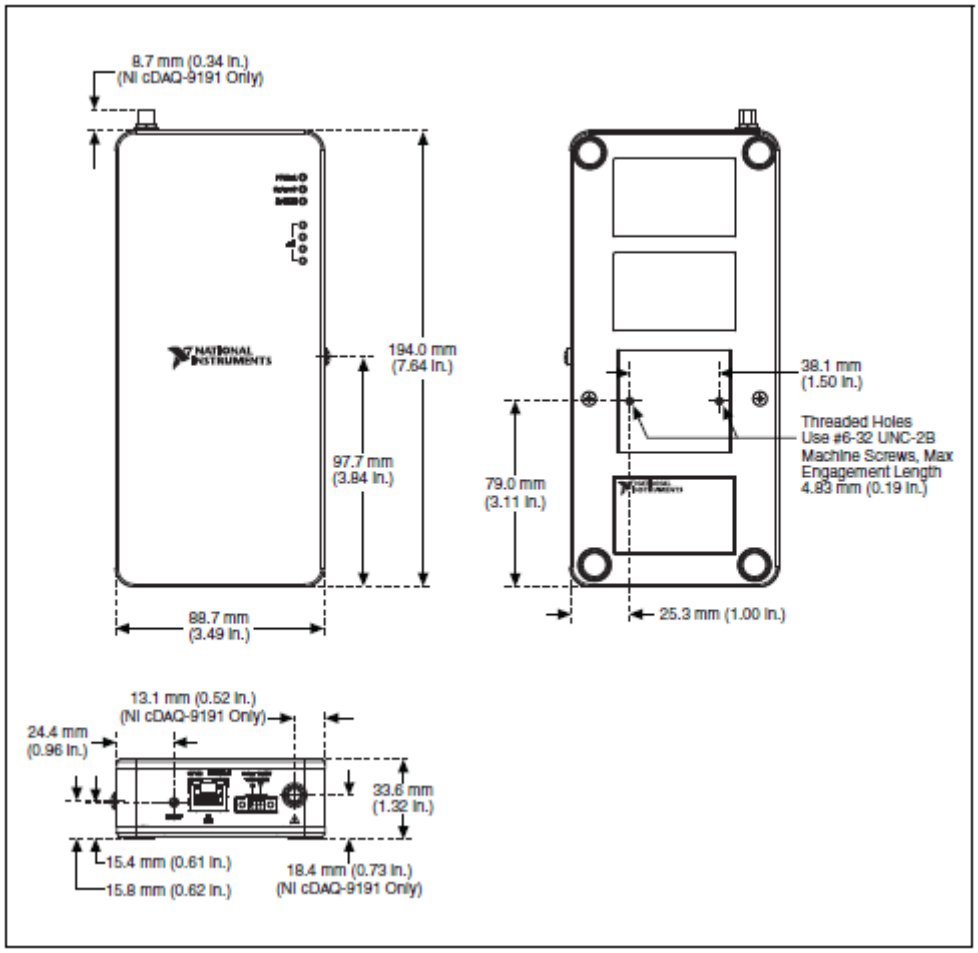
DC input characteristics

Level	Minimum	Maximum
Positive going threshold	1.43 V	2.28 V
Negative going threshold	0.86 V	1.53 V
Hysteresis	0.48 V	0.87 V

DC output characteristics

Level	Conditions	Minimum	Maximum
High	—	—	5.25 V
	Sourcing 100 µA	4.65 V	—
	Sourcing 2 mA	3.60 V	—
	Sourcing 3.5 mA	3.44 V	—
Low	Sinking 100 µA	—	0.10 V
	Sinking 2 mA	—	0.64 V
	Sinking 3.5 mA	—	0.8 V

Voltage input range	9 to 30 V
Maximum required input power	
NI cDAQ-9181	5 W
Weight (unloaded)	Approx. 470 g (16.6 oz)
Dimensions (unloaded)	194.0 × 88.7 × 33.6 mm (7.64 × 3.49 × 1.32 in.)



Operating Temperature (IEC-60068-2-1 and IEC-60068-2-2) NI cDAQ-9181/9191	0 to 55 °C
Storage Temperature (IEC-60068-2-1 and IEC-60068-2-2) NI cDAQ-9181/9191	–10 to 70 °C
Ingress protection	IP 30
Operating Humidity (IEC-60068-2-56)	10 to 90% RH, noncondensing
Storage	5 to 95% RH, noncondensing
Pollution Degree (IEC 60664)	2
Maximum altitude	5,000 m
Operational shock	30 g peak, half-sine, 11 ms pulse (Tested in accordance with IEC-60068-2-27.

This module meets the requirements of the following standards of safety for electrical equipment for measurement, control, and laboratory use:

- IEC 61010-1, EN 61010-1
- UL 61010-1, CSA 61010-1

NI-9481 Relay Module

The following specifications are typical for the range –40 to 70 °C unless otherwise noted.

Output Characteristics

Number of channels	4 electromechanical relay channels
Relay type	Single pole single throw (SPST)
Power-on output state	Channels off
Switching capacity (resistive load)	
Switching voltage	60 VDC max, 250 Vrms max
Switching current, per channel	
One channel on	4 A max at 30 VDC, 1 A max at 60 VDC, 4 A max at 250 Vrms
All channels on	2 A max at 30 VDC, 1 A max at 60 VDC, 2 A max at 250 Vrms
Resistance per channel, channel on	50 mΩ
Switching rate	1 operation per second
Relay release time	5 ms max
Relay operate time	10 ms max
Relay bounce time	3 ms
Off state leakage	10 µA max
Life expectancy	
Mechanical (no load)	20,000,000 operations
Electrical (connecting to load)	100,000 operations

Power Requirements

Power consumption from chassis	
Active mode	580 mW max
Sleep mode	5 mW max
Thermal dissipation (at 70 °C)	
Active mode	1.5 W max
Sleep mode	5 mW max
Screw-terminal wiring	12 to 24 AWG copper conductor wire with 10 mm (0.39 in.) of insulation stripped from the end
Torque for screw terminals	0.5 to 0.6 Nm (4.4 to 5.3 lb in.)
Ferrules	0.25 mm2 to 2.5 mm2
Weight	150 g (5.3 oz)

Safety Voltages

Connect only voltages that are within the following limits.

CHa-to-CHb	250 Vrms max, Measurement Category II

Hazardous Locations

U.S. (UL)	Class I, Division 2, Groups A, B, C, D, T4; Class I, Zone 2, AEx nC IIC T4

Safety Standards

This module meets the requirements of the following standards of safety for electrical equipment for measurement, control, and laboratory use:

- IEC 61010-1, EN 61010-1
- UL 61010-1, CSA 61010-1

Electromagnetic Compatibility

This module meets the requirements of the following EMC standards for electrical equipment for measurement, control, and laboratory use:

- EN 61326 (IEC 61326): Class A emissions; Basic immunity
- EN 55011 (CISPR 11): Group 1, Class A emissions
- AS/NZS CISPR 11: Group 1, Class A emissions
- FCC 47 CFR Part 15B: Class A emissions
- ICES-001: Class A emissions

CE Compliance

This product meets the essential requirements of applicable European Directives:

- 2006/95/EC; Low-Voltage Directive (safety)
- 2004/108/EC; Electromagnetic Compatibility Directive (EMC)

Shock and Vibration

Operating vibration, sinusoidal (IEC 60068-2-6)	5 g, 40 to 500 Hz; 0.062 in., double amplitude, 10 to 40 Hz

Environmental

National Instruments C Series modules are intended for indoor use only but may be used outdoors if installed in a suitable enclosure.

Operating temperature (IEC 60068-2-1, IEC 60068-2-2)	–40 to 70 °C
Storage temperature (IEC 60068-2-1, IEC 60068-2-2)	–40 to 85 °C
Ingress protection	IP 40

Operating humidity (IEC 60068-2-56)	10 to 90% RH, noncondensing
Storage humidity (IEC 60068-2-56)	5 to 95% RH, noncondensing
Maximum altitude	2,000 m
Pollution Degree (IEC 60664)	2

NI-9401 TTL I/O Module

The following specifications are typical for the range –40 to 70 °C unless otherwise noted. All voltages are relative to COM unless otherwise noted.

Input/Output Characteristics

Number of channels	8 DIO channels
Default power-on line direction	Input
Input/output type	TTL, single-ended

Digital logic levels

Input

Voltage	5.25 V max
High, VIH	2 V min
Low, VIL	0.8 V max

Output

High, VOH	5.25 V max
Sourcing 100 µA	4.7 V min
Sourcing 2 mA	4.3 V min

Low, VOL

Sinking 100 µA	0.1 V max
Sinking 2 mA	0.4 V max
I/O propagation delay	100 ns max
I/O pulse width distortion	10 ns typ
Input current (0 V ≤ Vin ≤ 4.5 V)	±250 µA typ
Input capacitance	30 pF typ
Input rise/fall time	500 ns max
Overvoltage protection, channel-to-COM	±30 V max on one channel at a time; however, continued use at this level will degrade the life of the module.

Power consumption from chassis

Active mode	580 mW max
Sleep mode	1 mW max

Thermal dissipation (at 70 °C)

Active mode	580 mW max
Sleep mode	1 mW max
Weight	145 g (5.1 oz)

Safety Standards

This module is designed to meet the requirements of the following standards of safety for electrical equipment for measurement, control, and laboratory use:

- IEC 61010-1, EN 61010-1
- UL 61010-1, CSA 61010-1

Hazardous Locations

U.S. (UL)	Class I, Division 2, Groups A, B, C, D, T4; Class I, Zone 2, AEx nC IIC T4
Canada (C-UL)	Class I, Division 2, Groups A, B, C, D, T4; Class I, Zone 2, Ex nC IIC T4
Europe (DEMKO)	EEx nC IIC T4

Environmental

National Instruments C Series modules are intended for indoor use only but may be used outdoors if installed in a suitable enclosure.

Operating temperature (IEC 60068-2-1, IEC 60068-2-2)	–40 to 70 °C
Storage temperature (IEC 60068-2-1, IEC 60068-2-2)	–40 to 85 °C
Ingress protection	IP 40
Operating humidity (IEC 60068-2-56)	10 to 90% RH, noncondensing
Storage humidity (IEC 60068-2-56)	5 to 95% RH, noncondensing
Maximum altitude	2,000 m
Pollution Degree (IEC 60664)	2

Operating vibration

Random (IEC 60068-2-64)	5 grms, 10 to 500 Hz
Sinusoidal (IEC 60068-2-6)	5 g, 10 to 500 Hz
Operating shock (IEC 60068-2-27)	30 g, 11 ms half sine, 50 g, 3 ms half sine, 18 shocks at 6 orientations

Electromagnetic Compatibility

This module is designed to meet the requirements of the following standards of EMC for electrical equipment for measurement, control, and laboratory use:

- EN 61326 EMC requirements; Industrial Immunity
- EN 55011 Emissions; Group 1, Class A
- CE, C-Tick, ICES, and FCC Part 15 Emissions; Class A

CE Compliance

This module meets the essential requirements of applicable European directives, as amended for CE markings, as follows:

- 2006/95/EC; Low-Voltage Directive (safety)
- 2004/108/EC; Electromagnetic Compatibility Directive (EMC)

Varian STAR 800 & 850 MIB Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501548
Revision D

Contents

Introduction 3
STAR 800 & 850 MIB Driver Installation 3
STAR 800 & 850 MIB Configuration 3
Defining and loading Ethernet parameters into an 850 MIB 5
Declaring an 850 MIB (Ethernet parameters already loaded in the MIB) 6
Buffering 6
Interface Supervisor 6
System Configuration 8
System using analog channel(s) and relay(s) 8
System using RS-232 port to control instrument 9
Diagnostics 10

Introduction

The STAR 800 & 850 MIB is an Ethernet enabled, analog-to-digital and serial communication interface between chromatographic instruments and the CompassCDS software. It enables the CompassCDS software to communicate with chromatographs without the need for a direct physical connection between CompassCDS computers and these instruments.

The STAR 800 & 850 MIB is used to either acquire analog input or digital (RS232) signals.

The STAR 800 & 850 MIB communicates with CompassCDS computers over a 10BaseT Ethernet configuration using TCP/IP protocol.

Several MIBs can be managed by the same CompassCDS computer(s). These interfaces must be declared and configured in the CompassCDS Configuration Manager as shown in the example below.

STAR 800 & 850 MIB Driver Installation

STAR 800 & 850 MIB driver installation is performed by launching STAR 800 & 850-MIB_Setup.exe on the station where CompassCDS software is installed.

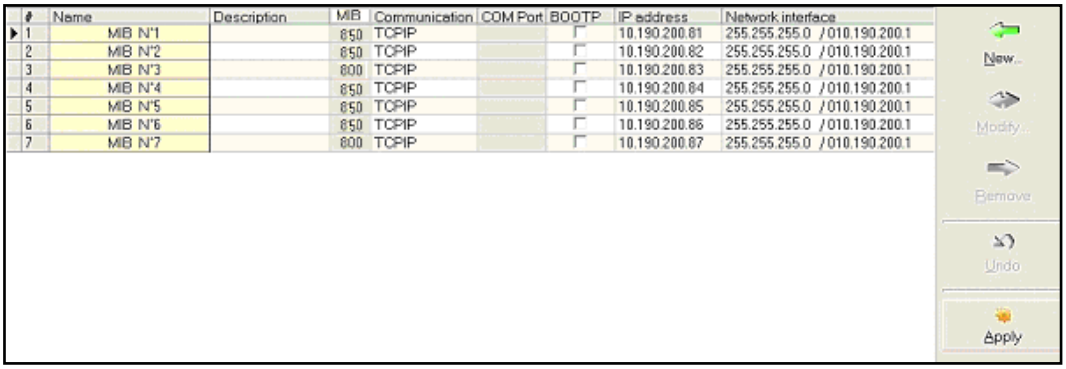
A serial number is required for the installation.

NOTE: The CompassCDS STAR 800 & 850 MIB driver can control both the legacy 800 MIB and the 850 MIB.

STAR 800 & 850 MIB Configuration

To configure the MIB on the CompassCDS computer, open the CompassCDS Configuration Manager, then select

in the Tools tab of the browser, or select the menu Option and click on Interface Configuration. This screen lists all the STAR 800 & 850-MIBs already configured, and allows the user to declare a new one.



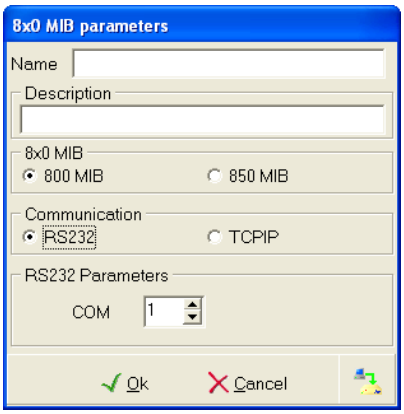
: to add an MIB

: to modify parameters of an existing MIB

: to remove an MIB that will be no longer used.

: to apply changes performed. Note that if you add a new MIB and forget to press the apply button, the MIB will not be available for use.

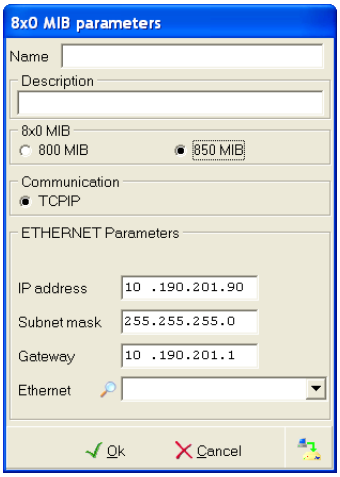
To add an MIB to the list, click on New. The following dialog box will be displayed:



Enter the Name of the STAR 800 & 850 MIB. This name will be used by CompassCDS to identify the STAR 800 & 850 MIB, and will be displayed in the driver configuration screen of an instrument using an MIB. This field must be filled in with a unique name.

The Description field may be entered to provide additional information about the MIB. It is not mandatory

Select the Interface type: 800 or 850 MIB.

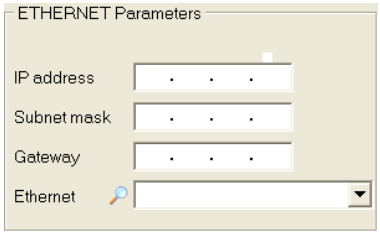


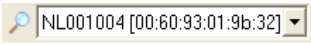
Only the TCP/IP configuration is then available.

The Ethernet parameters section enables the identification of the MIB. Each STAR 800 & 850 MIB must be assigned a unique IP address.

Defining and loading Ethernet parameters into a STAR 800 & 850 MIB

To define and load Ethernet parameters into a STAR 800 & 850 MIB, both the CompassCDS computer (where the configuration is to be performed) and the STAR 800 & 850 MIB must be connected into the same subnet and powered on



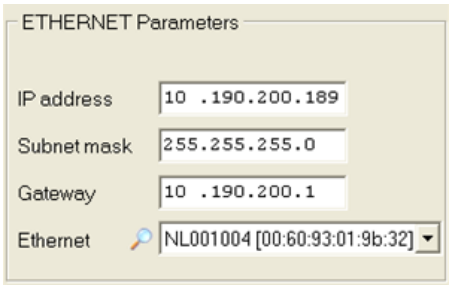
1. Select the MIB you want to configure by selecting its Ethernet address in the 

scrolling list. This scrolling list displays the Ethernet addresses of all connected STAR 800 & 850 MIBs.

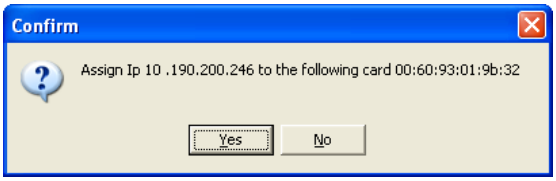
   Click on to refresh the list.

   Select the desired Ethernet address (if the desired STAR 800 & 850 MIB is not listed, reboot it and refresh the list).

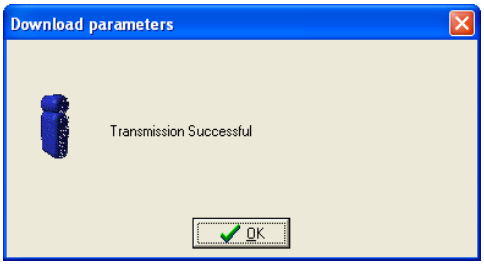
2. Enter the IP address, Subnet mask and (if required), a Gateway. These parameters are usually provided by a network administrator.



3. Click on to download the IP address and Subnet mask into the STAR 800 & 850 MIB. The following message is displayed:



   Click Yes. A successful message is displayed:



Click to validate the MIB configuration/declaration.

Declaring a STAR 800 & 850 MIB (Ethernet parameters already loaded in the MIB)

1. For a STAR 800 & 850 MIB configured within the same subnet as the CompassCDS acquisition and control computer:

   Click the button, then select the desired STAR 800 & 850 MIB from the scrolling Ethernet list. The IP address and the Subnet mask will be automatically filled in. It is up to user to define the Gateway.

2. For an STAR 800 & 850 MIB configured within a subnet to that of the CompassCDS acquisition and control computer:

   The STAR 800 & 850 MIB Ethernet address cannot be reached via the scrolling list. It is up to the user to manually enter a valid IP address, Subnet mask and Gateway for the STAR 800 & 850 MIB.

   In both cases, click to validate the MIB declaration.

Buffering

The STAR 800 & 850 MIB is fitted with 1 GB memory card. This card is designed to store analog acquisition points from connected chromatographic instruments, in cases where network communication between the STAR 800 & 850 MIB and the CompassCDS acquisition and control computer has been interrupted.

Interface Supervisor

The Interface Supervisor tool allows you to check the STAR 800 & 850 MIB state in real time. To start this tool in the CompassCDS Configuration Manager click on

or select the Options / Interface Supervisor menu.

Each MIB is represented by an interface symbol followed by its name.

For each STAR 800 & 850 MIB, the resources list [analog channels (ANALOG)], relays (RELAYS), RS-232 serial ports (RS-232) are also displayed, as well as the channel state:

Channel 1 : allocated channels are displayed in orange

Channel 2 : unallocated channels appear in green.

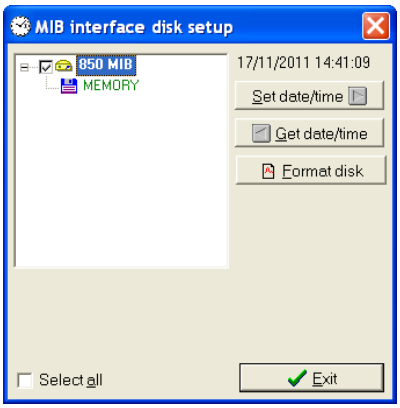
If the CompassCDS acquisition and control computer does not communicate with the interface (no physical connection to the network or to the RS-232 connector, power supply not connected, etc.), no channel will appear for this interface and its name will be preceded by a red cross: MIB.

For each STAR 800 & 850 MIB, it is also possible to display the following information by putting the mouse cursor onto the STAR 800 & 850 MIB name: Interface Type: STAR 800 & 850 MIB, the Mac address, the serial number, the IP address.

Click on to display the MIB list with details about connections (analog, relay).

Click on to display the MIB list in medium or reduced size, that is to say the MIB list and the channel number [e.g., analog (1/2) means that 2 analog channels are declared and that one is allocated] or only the MIB names.

Click to display information on the buffer card configuration.



Set date/time : to send the CompassCDS Station date/time into the STAR 800 & 850 MIB

Get date/time : to display the date/time stored in the STAR 800 & 850 MIB

Format disk : to format information stored on the card

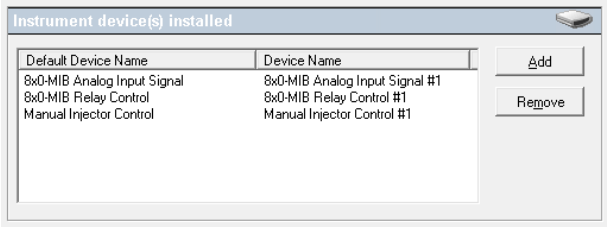
The button updates the Supervisor if pressed.

System Configuration

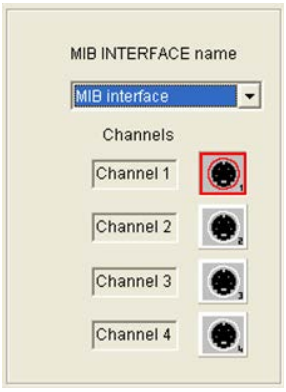
System using analog channel(s) and relay(s)

To configure a system using both analog input channels and relay(s) outputs on an STAR 800 & 850 MIB, follow these instructions:

1. Configure the STAR 800 & 850 MIB using the Interface Configuration tool.
2. Create the instrument. In the list of devices screen, select and add the STAR 800 & 850-MIB Analog Input Signal and the STAR 800 & 850-MIB Relay Control drivers:

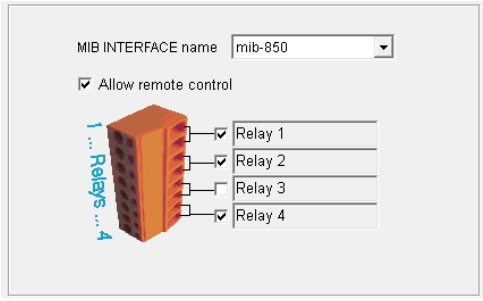


3. In the configuration screen, select the STAR 800 & 850 MIB and define the STAR 800 & 850 MIB and the desired analog channel(s) by clicking on the desired channel icon:



The previous picture represents an STAR 800 & 850 MIB fitted with two 2-channel ADC cards, i.e., 4 channels in total. Selected channels will appear as red and it is possible to modify the Channel name for each selected channel. The channel positions on the 800 MIB appear as follows:

4. In the configuration screen, select the STAR 800 & 850 MIB Relays Control icon, define the STAR 800 & 850 MIB, and select the desired relay(s) to be controlled. It is possible to modify the relay descriptions in this screen.



System using RS-232 port to control instrument

To configure a system controlled via an STAR 800 & 850 MIB serial port (RS232), follow the instructions:

1. Configure the STAR 800 & 850 MIB using the Interface Configuration tool.

2. Create the instrument. In the list of devices screen, select the instrument driver that is connected to the STAR 800 & 850 MIB via the serial port (RS232).
3. In the system configuration screen, select the module/Instrument screen, then select the STAR 800 & 850 MIB and the serial port (ex: Valco Valves, CTC Combi PAL).

Diagnostics

If an MIB is preceded by a red cross in the supervisor:

1. Verify that the interface is switched ON.
2. Verify that the IP address captured in Interface configuration is correctly entered, and that it corresponds to the IP address of the interface.
3. Verify that a valid Ethernet cable connection exists between the interface and the hub (or wall plug).
4. If the interface is still not detected, re-program the network parameters of the interface.

If the above steps do not solve the communication problem, please contact Scion Instruments Technical Support.

Varian STAR 850 MIB
Instrument User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501549
Revision D

Contents

Introduction ..... **Error! Bookmark not defined.**
8x0 MIB Driver Installation ..... **Error! Bookmark not defined.**
8x0 MIB Configuration ..... **Error! Bookmark not defined.**
Defining and loading Ethernet parameters into an 850 MIB ..... **Error! Bookmark not defined.**
Declaring an 850 MIB (Ethernet parameters already loaded in the MIB) ..... **Error! Bookmark not defined.**
Buffering ..... **Error! Bookmark not defined.**
Interface Supervisor ..... **Error! Bookmark not defined.**
System Configuration ..... **Error! Bookmark not defined.**
System using analog channel(s) and relay(s) ..... **Error! Bookmark not defined.**
System using RS-232 port to control instrument ..... **Error! Bookmark not defined.**
Diagnostics ..... **Error! Bookmark not defined.**

Introduction

This document describes the 850 MIB and the associated extension cards.

NOTE: The socket-outlet shall be installed near the equipment and shall be easily accessible.

This is a Class A product.

In a domestic environment this product may cause radio interference in which case the user may be required to take adequate measures.

Front View

Status light

Orange: Starting up or shutting down.

Green: Ready.

Run light

Blue: The remote workstation is connected.

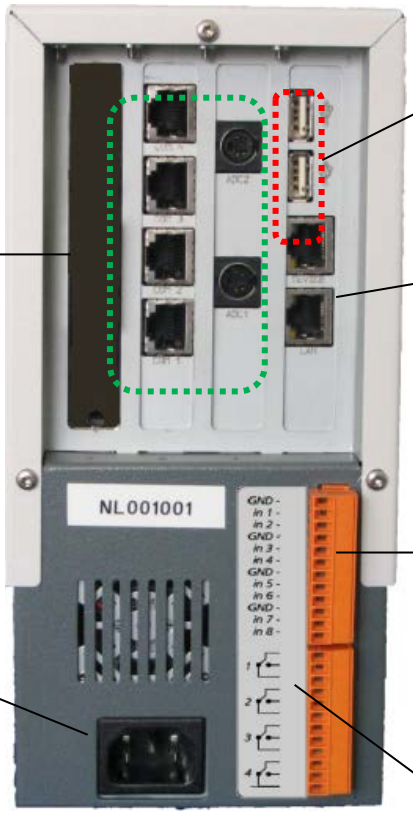
Infra-Red sensor

Not used

On/Off button

- Press once to start up the device,
- Press for around 2 seconds (until the status light turns orange) to soft shut down the device,
- Pressing for more than 5 seconds will force a hard shut down.

Rear View



Additional extension ports
2 USB ports and 1 Ethernet port. Not used.

Extension cards
Connection to instruments. See next section for details.

LAN
10/100 Mbps Ethernet connection.

Synchronization Inputs
Active when In X is connected to GND or a 5V voltage is applied.

Power
Connect to **90~265V AC**, **47~63Hz** network.

4 Relays
With normally closed and normally opened contacts.

The limits for the relays contacts are: **30V AC/DC**, **2.5A** (protected with fuses).

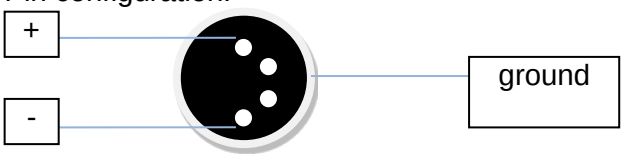
Extension cards

There are three extension slots that can receive combinations of the following extension cards.

The extension cards provide the interface to the analytical instruments.

2-Channel ADC Converter Card

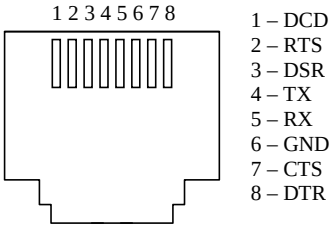
Pin configuration:



Differential input voltage limits -12V / +12V.

4-Port Serial Card

Pin configuration:

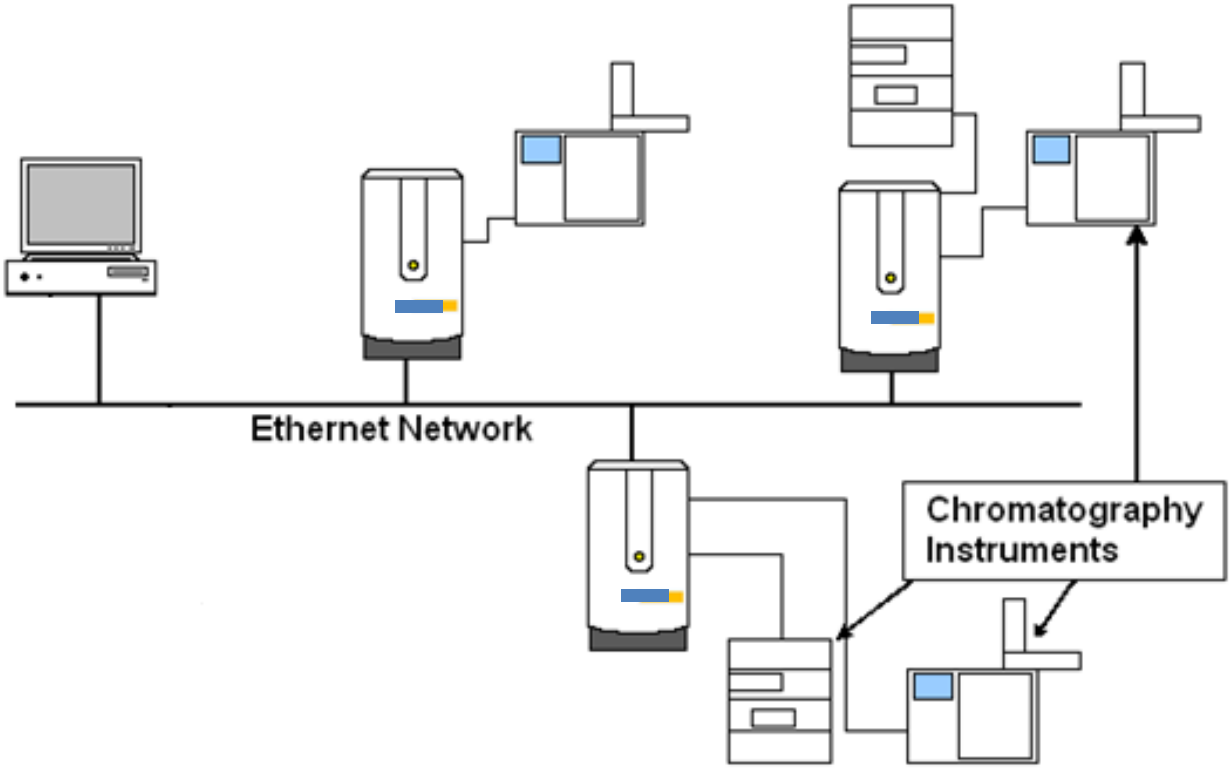


Maximum baud rate 115200 baud.

Environment

The MIBs provide access to chromatographic instruments that have analog outputs or RS-232 communication, either by direct connection to a PC or across TCP/IP networks

The MIBs are controlled via CompassCDS software.



Specifications

Physical	Number of board slots	3 PCI internal connections
	Maximum number of ADC channels	4
	Maximum number of serial connections	8
	Power supply	110 to 250 VAC, 50 to 60 Hz autosensing
	Dimensions	5.1 (w) x 9.0 (h) x 9.3 in. (d) (13.0 x 22.8 x 23.5 cm)
	Weight	6.8 lb (3.1 kg)
	Shipping weight	9.9 lb (4.5kg)
System	Start inputs	4 contact closures
	Contact closure output relays	4
	USB connections	2 for future use
	Ethernet connections	2 (1 for network connection & 1 for future use)
	System memory	1Gb flash memory for firmware & analog data storage
ADC Board	Number of ADC channels	2 asynchronous per board
	ADC ranges	+/- 1VFS, +/- 2.5 VFS, +/- 10VFS
	ADC range control	Software
	Electronic noise	<1 µV at 1 VFS, 10 points/sec
	Channel crosstalk	<1 µV
	Data rate	1 to 100 Hz
	ADC resolution	24 bit
	Dynamic range	> 1000,000:1
	Common mode rejection ratio	1 V range, <90 db
	Maximum input voltage without damage	+/- 12V
	Data buffering	1 Gb compact flash memory (300 h at 100 Hz)
Serial Board	Serial interfaces	4 independent per board
	Serial protocol	RS-232
	Data rate	110 to 19200 Bd
Ethernet	Data rate	10/100 MHz
	Hardware	10/100 Base T with RJ45 connector
	Protocol	TCP/IP

Agilent 5890 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501551
Revision C

Contents

Introduction 3
Installation and Configuration 3
Installing the Driver Software 3
Configuring the Driver 3
Configuring the Agilent Technologies 5890 Gas Chromatograph 3
Building a Method 6
Creating a New Method 6
Control Method Section for the Agilent 5890 Gas Chromatograph 8
Valves Control 9
Inlet Control 9
Standard Inlet 10
PCOC Inlet 11
Column control 11
Oven Control 14
Cryo Control 15
Detector Control 15
Aux Control 17
Events Control 19
General Control 20
Starting and Viewing an Acquisition 21
Quick Start and Sequence 21
Quick Start (Single Acquisition) 21
Sequence 22
Running Acquisition Status 23
Viewing a Running Acquisition 23
Status of the Agilent 5890 Gas Chromatograph 23
Appendix 26
Injection Volumes 26
Configuring a 5890 GC to CompassCDS 27
Setting and Configuration 29
Wiring Connections between CompassCDS and the 5890 GC with Autosampler 30
Agilent 5890 GC with 6890 Autosampler Controller Connected to MIB-interface COM ports 30
Agilent 5890 GC with 6890 Autosampler Controller Connected to PC COM ports 32
Agilent 5890 GC with 7673 Autosampler Controller Connected to MIB-interface COM ports 33
Agilent 5890 GC with 7673 Autosampler Controller Connected to PC COM ports 35

Introduction

This document describes the configuration of the Agilent Technologies 5890 GC driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS Installation Guide.

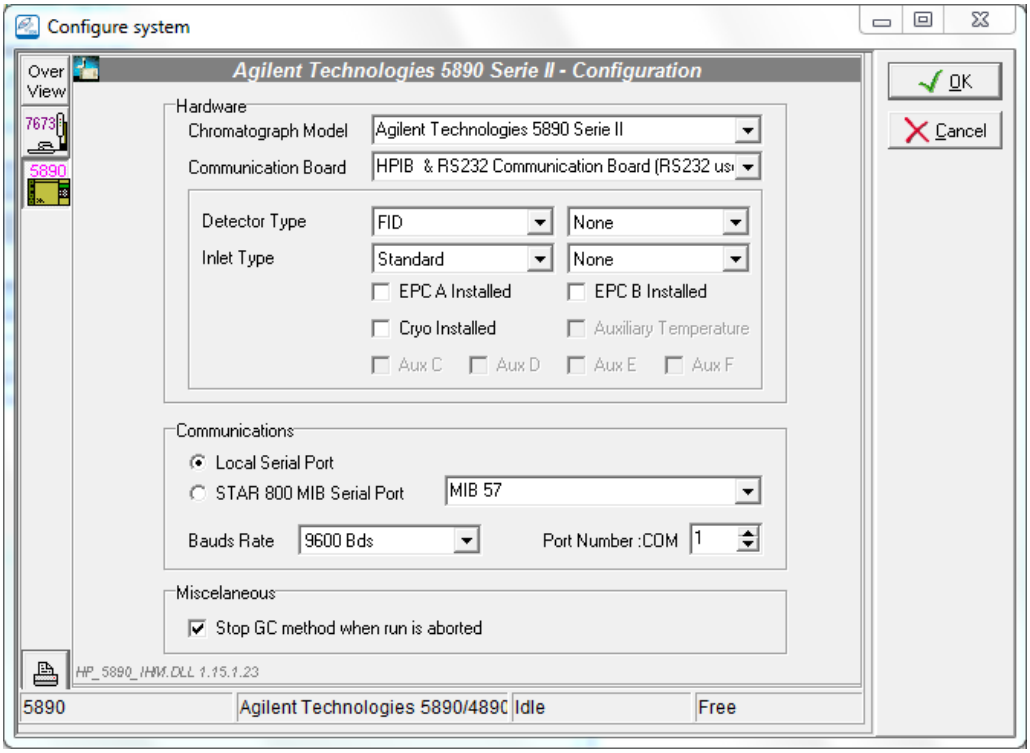
Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Agilent Technologies 5890 Gas Chromatograph

Click on the

button corresponding to the Agilent Technologies 5890 Gas Chromatograph driver and the configuration screen appears:



Hardware Parameter Group

Chromatograph Model:

Select the Chromatograph Model. The available models are: Agilent Technologies 4890A, Agilent Technologies 4890D, Agilent Technologies 5890 Series I, Agilent Technologies 5890 Series II and Agilent Technologies 5890 Series II +.

Communication Board:

Choose HPIB and RS232 Communication Board (RS232 used) in the list. The HPIB and RS 232 Communication Board (HPIB used) is not implemented and the Simple RS232 Communication Board is not recommended.

NOTE: Refer to the *Appendix* to learn more about the cables needed for the GC connection to the MIB-interface.

Detector Type:

The left scrolling list allows you to select the front detector. The right scrolling list allows you to select the back detector. The available choices are: None, ECD, FID, NPD, TCD, and FPD.

Inlet type:

The left scrolling list allows you to select the front inlet. The right scrolling list allows you to select the back inlet.

The available choices are: None, Standard, and PCOC. PCOC stands for Programmable Cool On-Column.

EPC A installed:

Check this box if the Electronic Pressure Control option is installed for the front inlet. This option is available only for the Agilent Technologies 5890 Series II and Series II +.

EPC B installed:

Check this box if the Electronic Pressure Control option is installed for the back inlet. This option is available only for the Agilent Technologies 5890 Series II and Series II +.

Cryo installed:

Check this box if the cryogenic oven option is installed. This option is available only for the Agilent Technologies 5890 Series II and Series II +.

Auxiliary Temperature:

Check this box if an auxiliary temperature option is installed. This option is available only for the Agilent Technologies 5890 Series II +.

Aux C, Aux D, Aux E and Aux F:

Check the corresponding box(es) if the auxiliary electronic pressure control option is installed. This option is available only for the Agilent Technologies 5890 Series II+.

Communications Parameter Group

Local Serial Port:

Select this option if the chromatograph is directly connected to the PC.

Star 800 & 850 MIB Serial Port:

Select this option and then the name of the MIB-interface used to connect to the chromatograph.

NOTE: If you will use the serial port installed in the MIB-interface, configure the MIB-interface before configuring the Agilent Technologies 5890 Gas Chromatograph driver.

Bauds Rate:

Choose 9600 Bds.

Port Number: COM:

Select the PC or STAR 800 & 850 MIB-interface Serial port number to which the chromatograph will be connected.

Miscellaneous Parameter Group

Stop GC method when run is aborted:

Check this box if you want the instrument to immediately return to the initial conditions after aborting a run. All current programs will also be aborted.

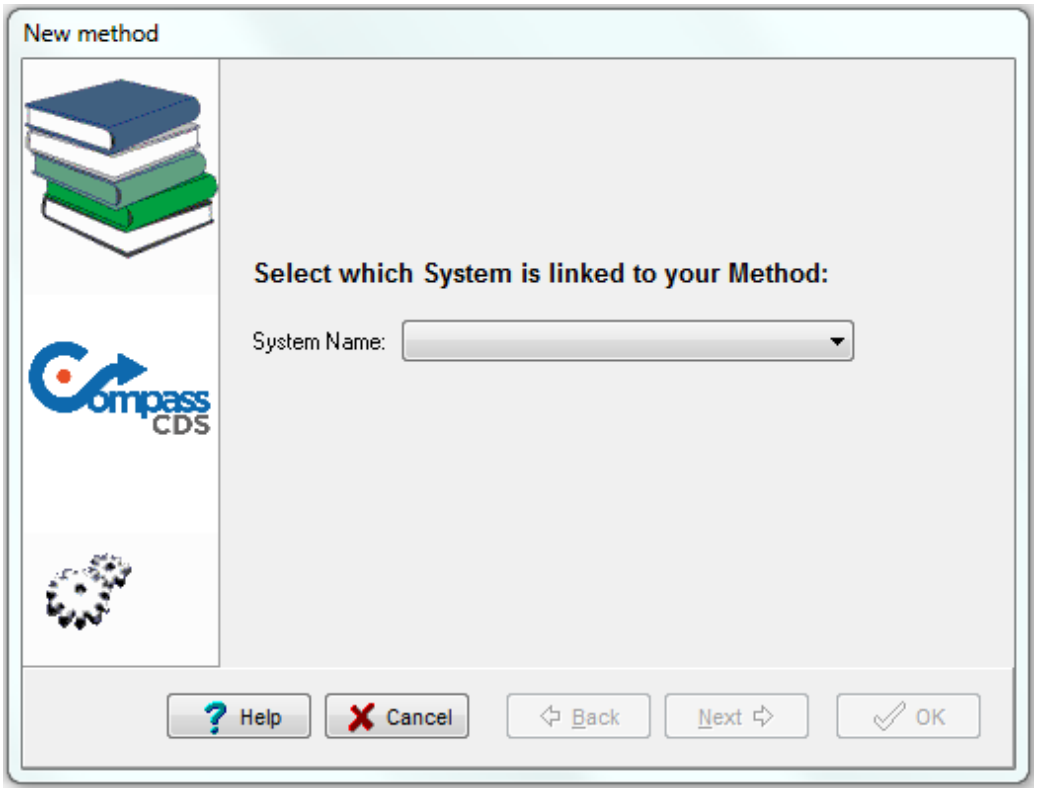
Building a Method

Creating a New Method

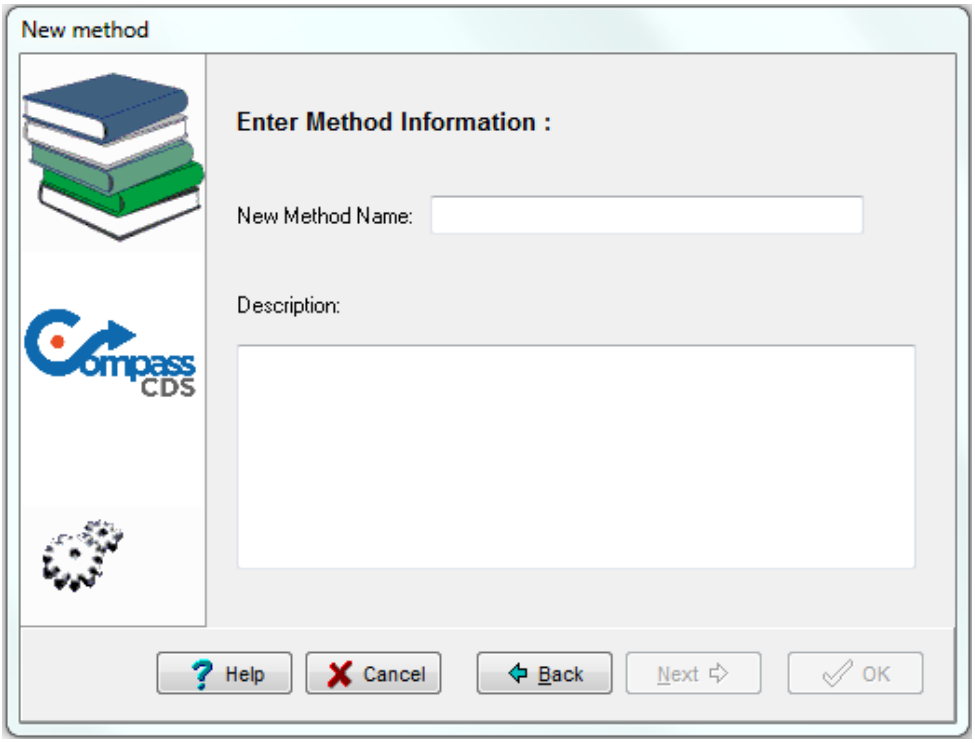
The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

1. To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS Chromatography Data System main menu.

   A wizard guide will appear and provide assistance during the first steps of method creation:



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.
3. Once this field is completed, click on the Next button to move to the second step of the method creation:



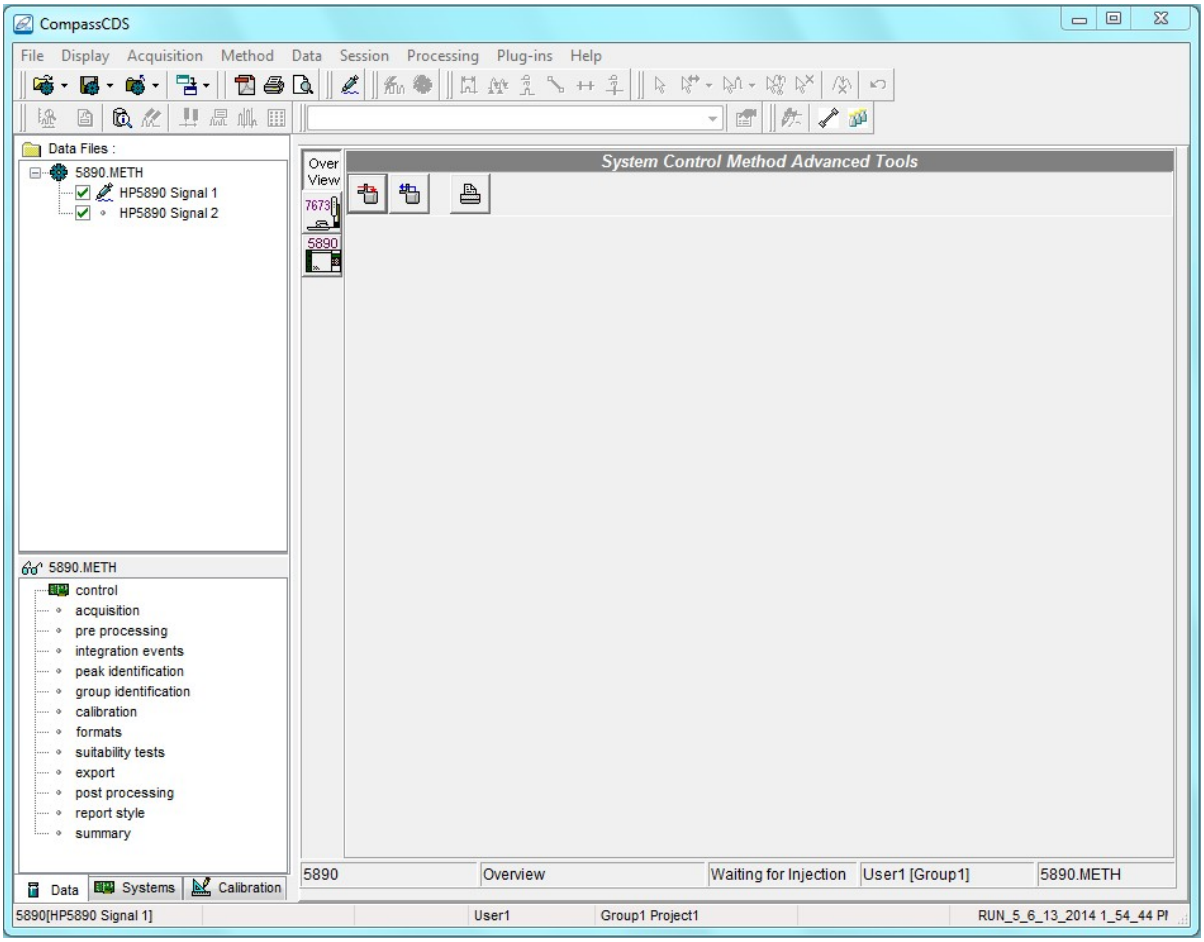
4. Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).
5. Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

The control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Agilent 6890 Gas Chromatograph is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to the CompassCDS User Guide.

Control Method Section for the Agilent 5890 Gas Chromatograph

Once the new method is created, select the control section in the lower part of the browser. The following screen appears:



Press the Over View button to display the ***System Control Method Advanced Tools*** window:

to send the current method to the instrument

to get the active method from the instrument

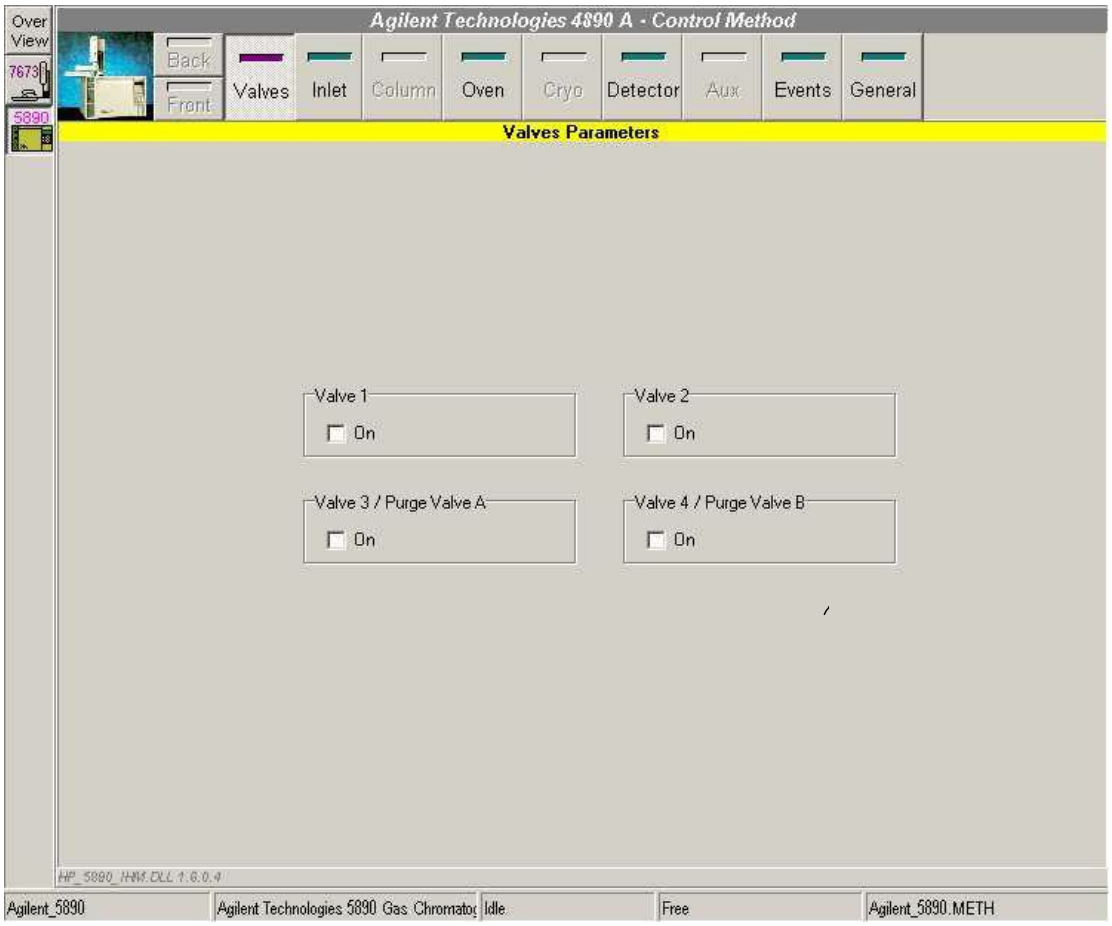
to print the current method

Click on the 5890 button to display the Agilent 5890 Gas Chromatograph control method section.

It contains four sub-sections which are always active: Valves, Oven, Events and General. Up to five additional sub-sections can be also activated depending on the system configuration: Inlet (if at least one inlet has been configured), Column (if EPC A or/and EPC B have been configured), Cryo (if Cryo has been configured), Detector (if at least one detector has been

configured) and Aux (if Auxiliary Temperature, Aux C, Aux D, Aux E or Aux F have been configured), and Valves (if Valves have been configured). Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Valves Control



Check the box corresponding to the valve to switch it *On*. Valve 1 manages a relay.

Valve 2 manages a relay.

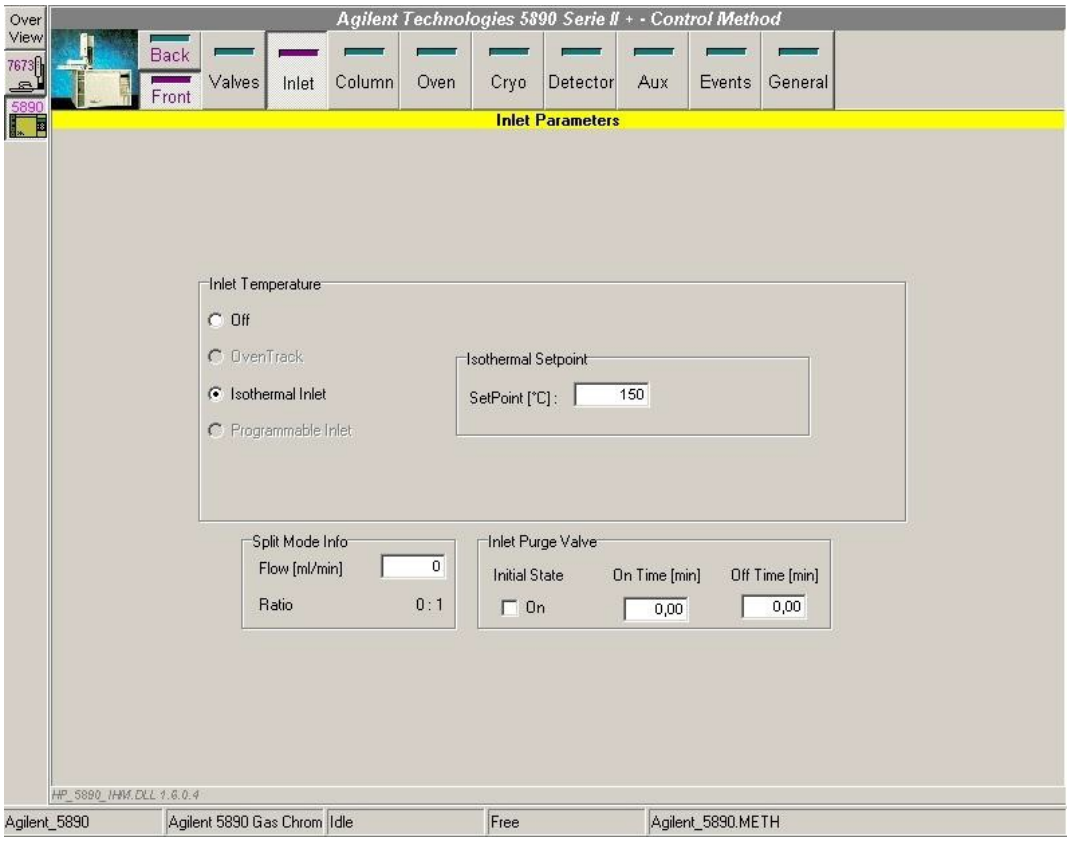
Valve 3 manages the splitless injection purge of the front inlet. Valve 4 manages the splitless injection purge of the back inlet.

NOTE: For Valve 3 and Valve 4, there is a link between the Valves window and the Inlet window. For instance, if Valve 3 is checked in the Valve window, the Inlet Purge Valve box in the Front Inlet window will be automatically checked. If the Inlet Purge Valve box in the Front Inlet window is checked, then Valve 3 will be automatically checked in the Valve window.

Inlet Control

Depending on the system configuration, the Inlet sub-section contains one or two inlets: Front and/or Back. The activated fields also depend on the system configuration. Click on the inlet to edit (Front or Back).

Standard Inlet



Inlet Temperature Parameter Group

Select Off to turn off the inlet heater.

Select *Isothermal Inlet* to have a constant inlet temperature. Enter the setpoint value in the *Isothermal Setpoint* field.

Split Mode Info Parameter Group

This parameter group appears only when an EPC option is configured on the corresponding inlet. Enter the split flow rate in the Flow field.

The *Ratio* is a read only field, automatically calculated according to the split flow and column flow.

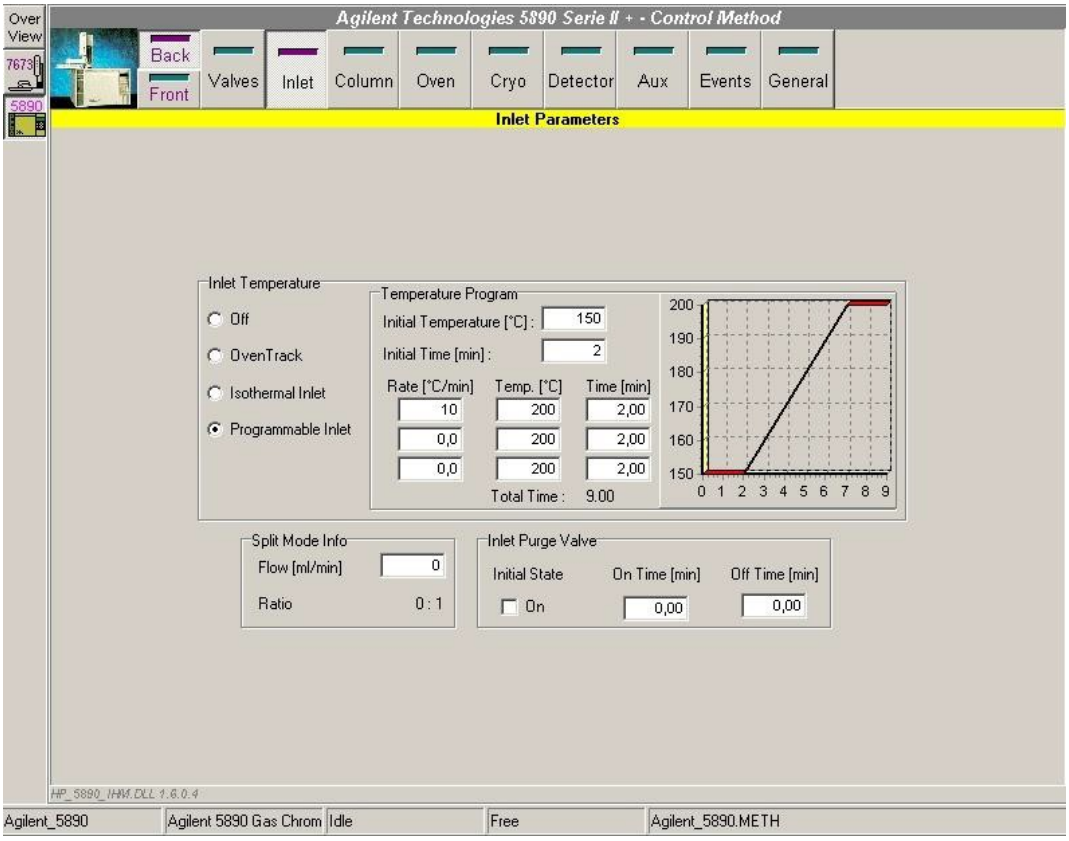
Inlet Purge Valve Parameter Group

Check *Initial state On* to turn the valve On (split mode) in the initial state. Enter the *On Time* and *Off Time* values during which the valve remains open.

The allowed range is 0 to 655 minutes but only the values which are lower than the run time will be taken into account. If both times are set to 0, the valves remain always open.

By default, the injection is realized in splitless mode (the *Initial State* box is unchecked).

PCOC Inlet



Inlet Temperature Parameter Group

Select *Off* to turn off the inlet heater.

Select *OvenTrack* to have the inlet temperature profile exactly like the column oven temperature profile.

Select *Isothermal Inlet* to have a constant inlet temperature. Enter the setpoint value in the *Isothermal Setpoint* field. Check *Programmable Inlet* to program the inlet temperature.

In the *Initial Temperature* field, enter the inlet initial temperature. In the *Initial Time* field, enter the time for this first plateau.

In the table program the rates, the plateau temperatures, and the time duration of the inlet plateau temperature. The total time of the inlet program is displayed in the *Total Time* field.

The graph to the right side of the table displays the inlet temperature program.

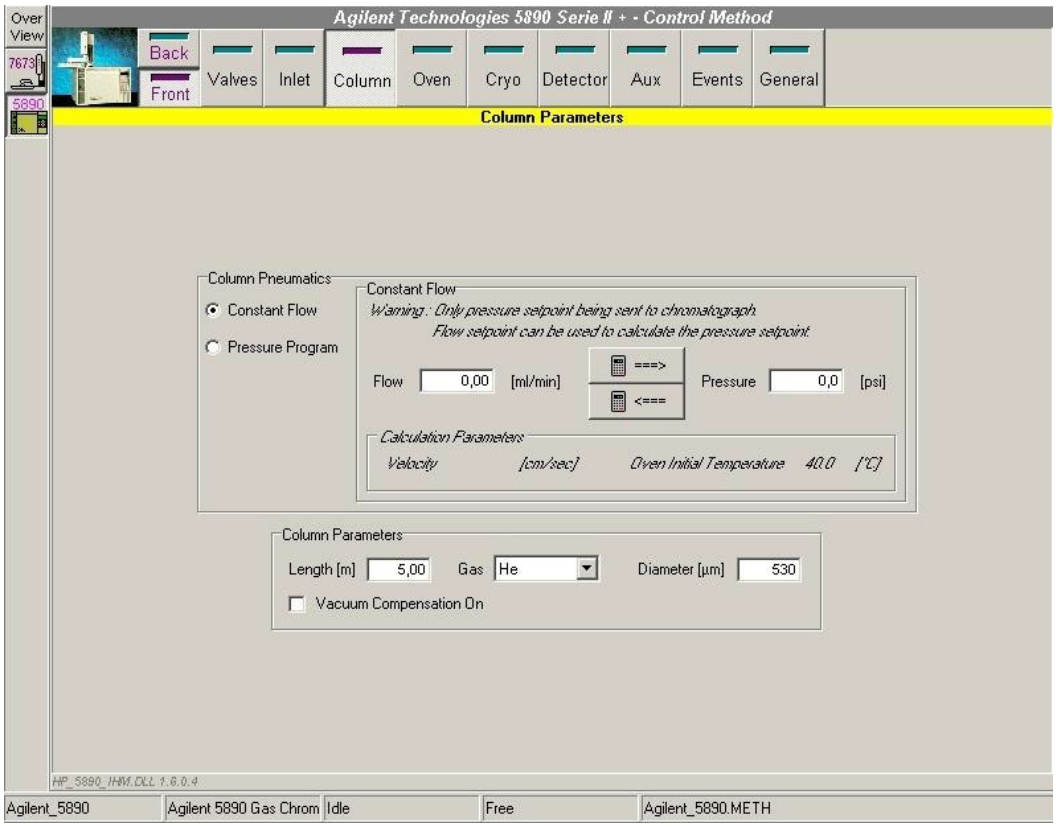
NOTE: The *Split Mode Info* and *Inlet Purge Valve* fields are inactive with an on-column inlet.

Column control

This sub-section is active only when an EPC is configured for the system in the CompassCDS Configuration Manager. In this case a *Constant flow* or a *Pressure program* can be entered.

The *Front* and *Back* and buttons allow you to specify the parameters for the two columns.

Constant flow



Column Pneumatics Parameter Group

Check *Constant Flow* to have a constant flow in the column. To maintain a constant flow, the pressure changes according to the oven temperature program.

Enter the *Flow* or the *Pressure* and click on or to calculate the corresponding pressure or flow.

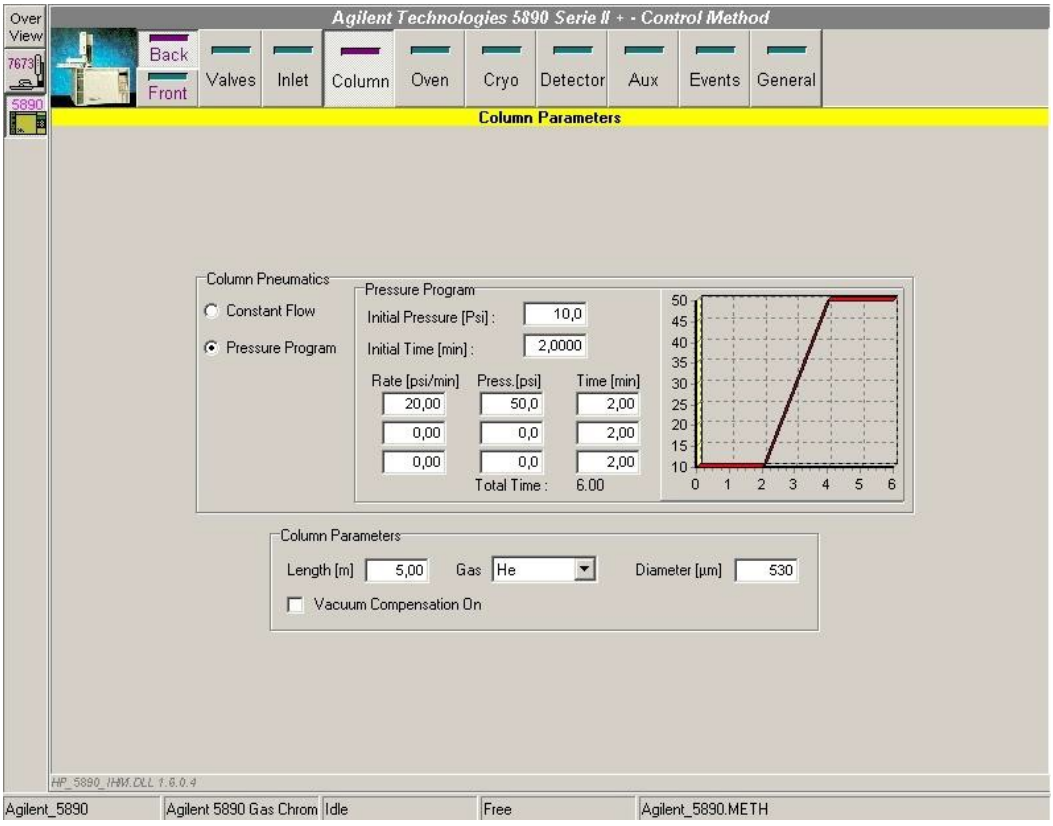
The *Velocity* and *Oven Initial Temperature* are a read-only display. The *Oven Initial Temperature* is displayed according to the *Initial Temperature* field of the *Oven* Tab.

Column Parameters Parameter Group

Enter the column *Length*, *Gas*, and *Diameter* in the corresponding fields. If these parameters and the *Oven Initial Temperature* are modified after the pressure calculation, click on the button again to update the column specification.

Check the *Vacuum Compensation On* box if the chromatograph is connected to a mass spectrometer, to correct the output pressure.

Program Pressure



Column Pneumatics parameter group

Check Pressure Program.

In the *Initial Pressure* field, enter the column initial pressure. In the *Initial Time* field, enter the time for this first plateau.

In the table program the rates, the plateau pressure, and duration of the plateau pressure. The total time of the column program is displayed in the *Total Time* field.

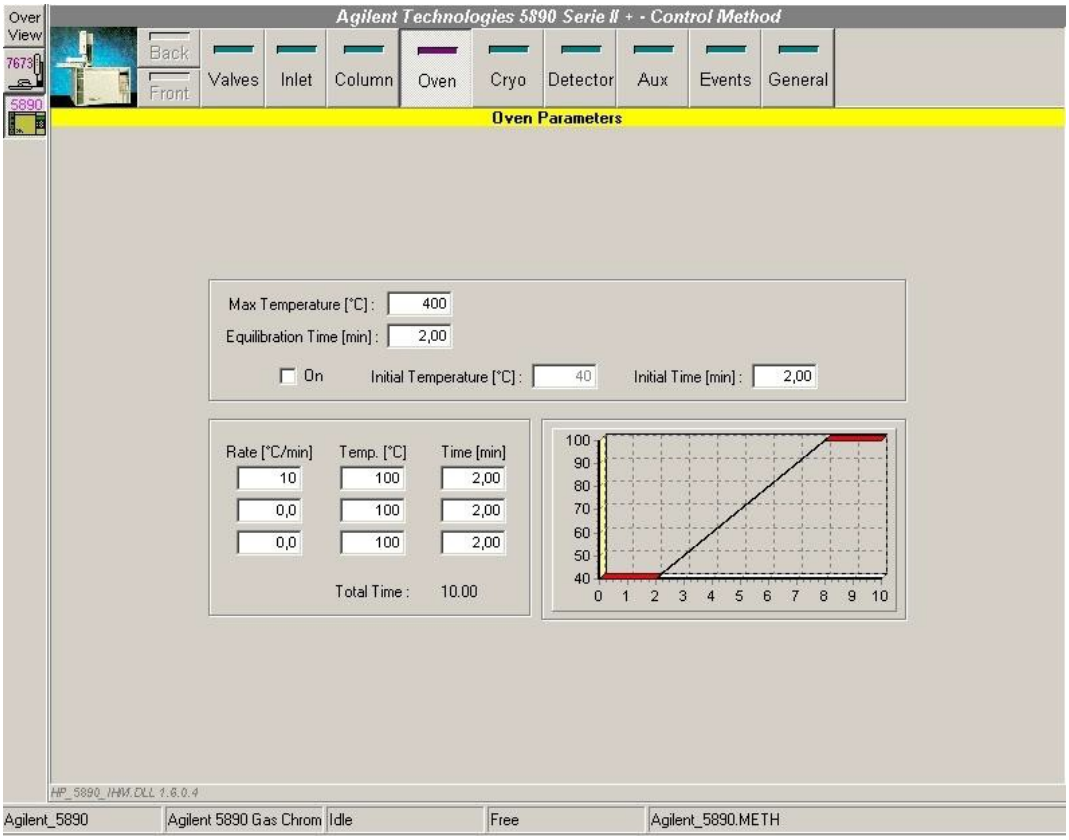
The graph to the right of the table displays the pressure program.

Column Parameters parameter group

Enter the column *Length*, *Gas*, and *Diameter* in the corresponding fields.

Check the *Vacuum Compensation On* box if the chromatograph is connected to a mass spectrometer, to correct the output pressure.

Oven Control



In the *Max Temperature* field, enter the column maximum temperature.

In the *Equilibration Time* field, enter the time before the GC becomes Ready. Check the *On* box to activate the oven temperature program.

In the *Initial Temperature* field, enter the oven initial temperature. In the *Initial Time* field, enter the time for this first plateau.

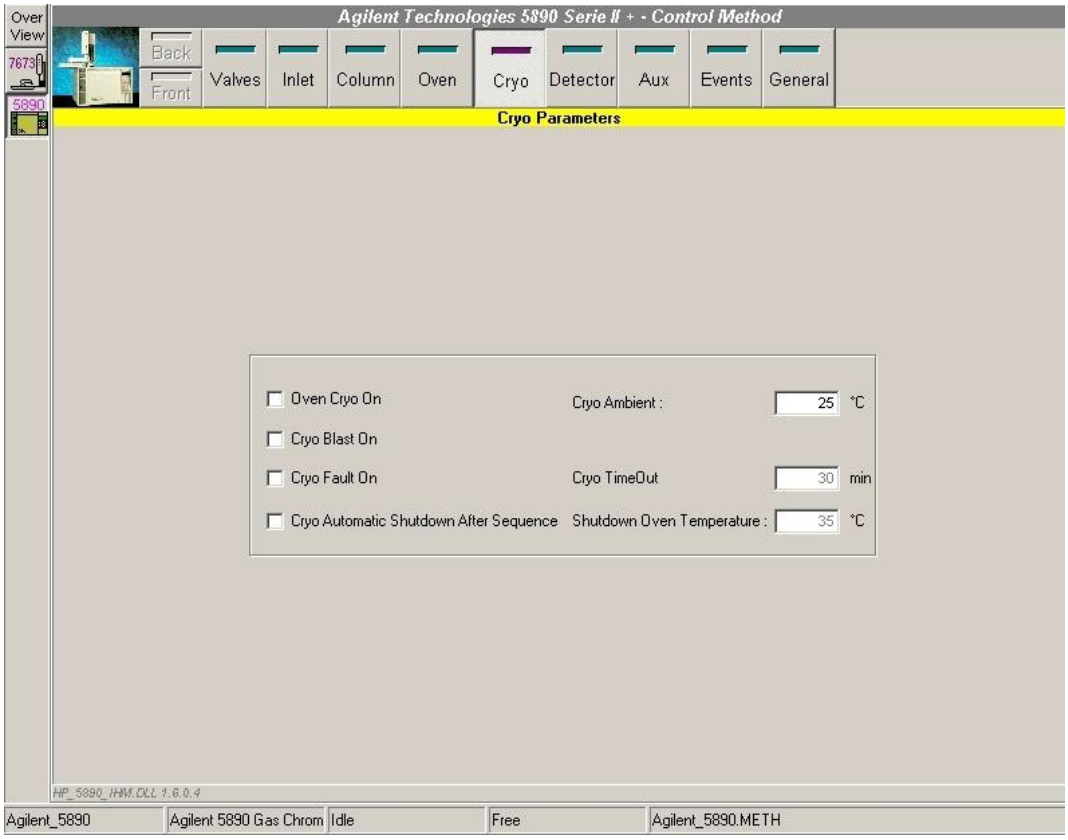
In the table program the rates, the plateau temperatures, and the duration of the column oven plateau temperature. The total time of the oven program is displayed in the *Total Time* field.

The graph to the right side of the table displays the oven temperature program.

Cryo Control

This sub-section is active only when a Cryogenic option is configured for the system in the CompassCDS Configuration Manager.

Click on the *Cryo* button, the *Cryogenic Parameters* screen appears. The cryogenic system generates an oven temperature lower than the ambient temperature. The fields shown depend on the configuration.



Check the *Oven Cryo On* box to activate the cryogenic system. Enter the ambient temperature in the *Cryo Ambient* field.

Check *Cryo Blast On* to quickly cool the oven after a run.

Check *Cryo Fault On* to stop the oven after 17 minutes if the cryogenic system has not reached the desired temperature. The oven stops if no injection is started before the time entered in the *Cryo Timeout* field.

Check *Cryo Automatic Shutdown After Sequence* to stop the cryogenic system use at the end of a sequence. In the

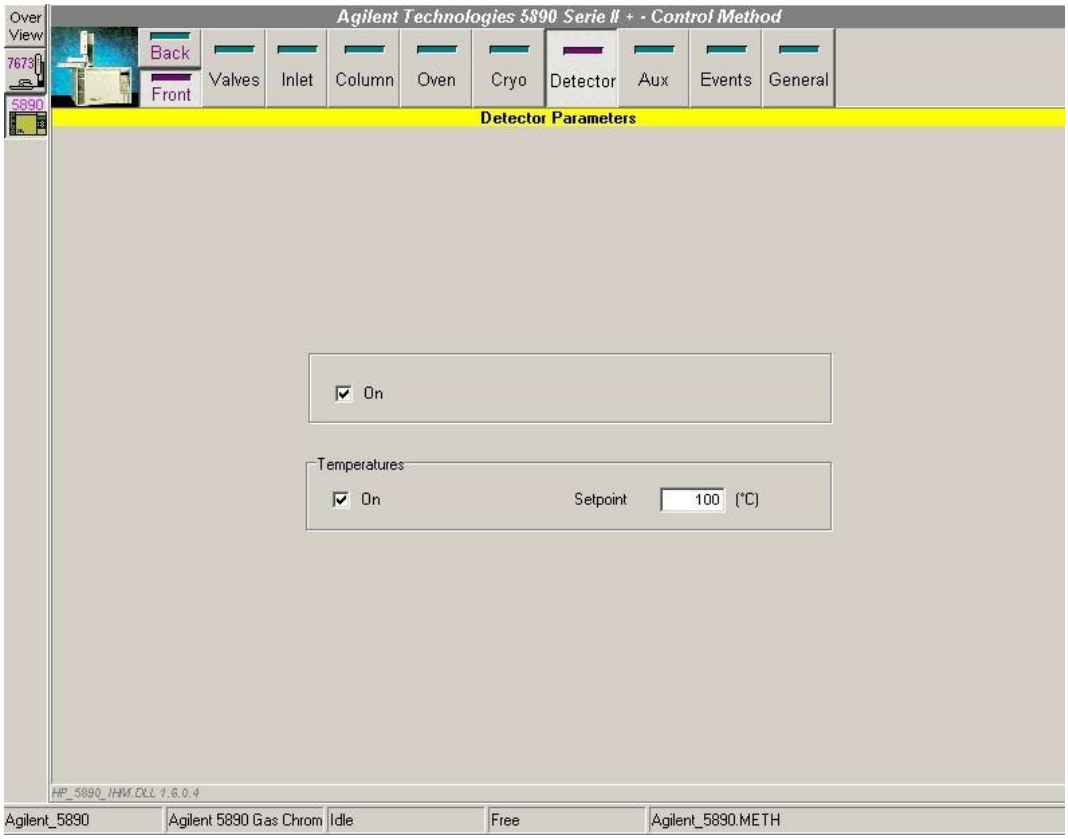
Shutdown Oven Temperature field, enter the temperature the oven has to reach at the end of the sequence.

Detector Control

Click on the *Front* or *Back* buttons to enter the parameters for each installed detector.

FID (Flame Ionization Detector), ECD (Electron Capture Detector), FPD (Flame Photometric Detector) and NPD (Nitrogen-Phosphorous Detector)

For these four detectors, the available parameters to be set are identical.

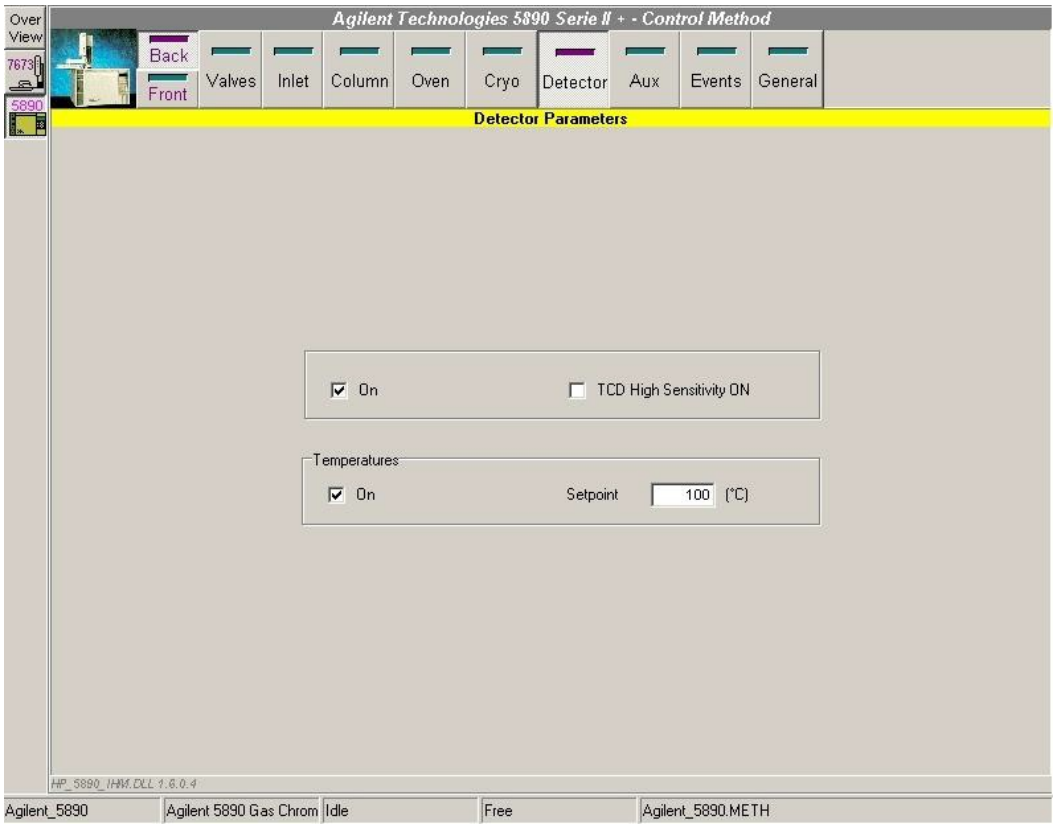


Check *On* to activate the detector.

Temperatures parameter group

Check *On* to set the detector temperature in the *Setpoint* field.

TCD (Thermal Conductivity Detector)



Check *On* to activate the detector.

Check *TCD High Sensitivity ON* when the analyzed compound concentration is lower than 10%. The signal is saturated when the concentration is greater.

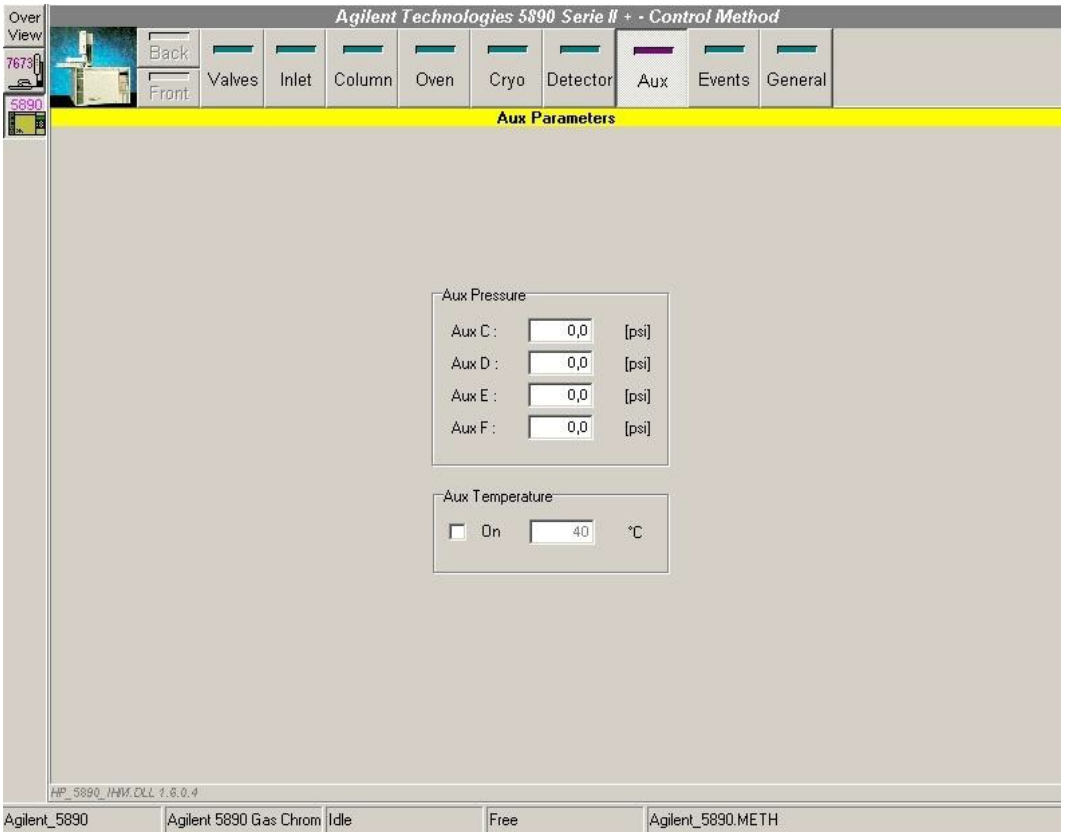
Temperatures parameter group

Check *On* to set the detector temperature in the *Setpoint* field.

Aux Control

The Agilent 5890 Series II+ gives the choice to have an extra heating block and four auxiliaries (*Aux C*, *D, E*, and *F*).

This sub-section is active only when at least one auxiliary is configured for the system in the CompassCDS Configuration Manager. The different fields depend on system configuration.



Aux Pressure Parameter Group

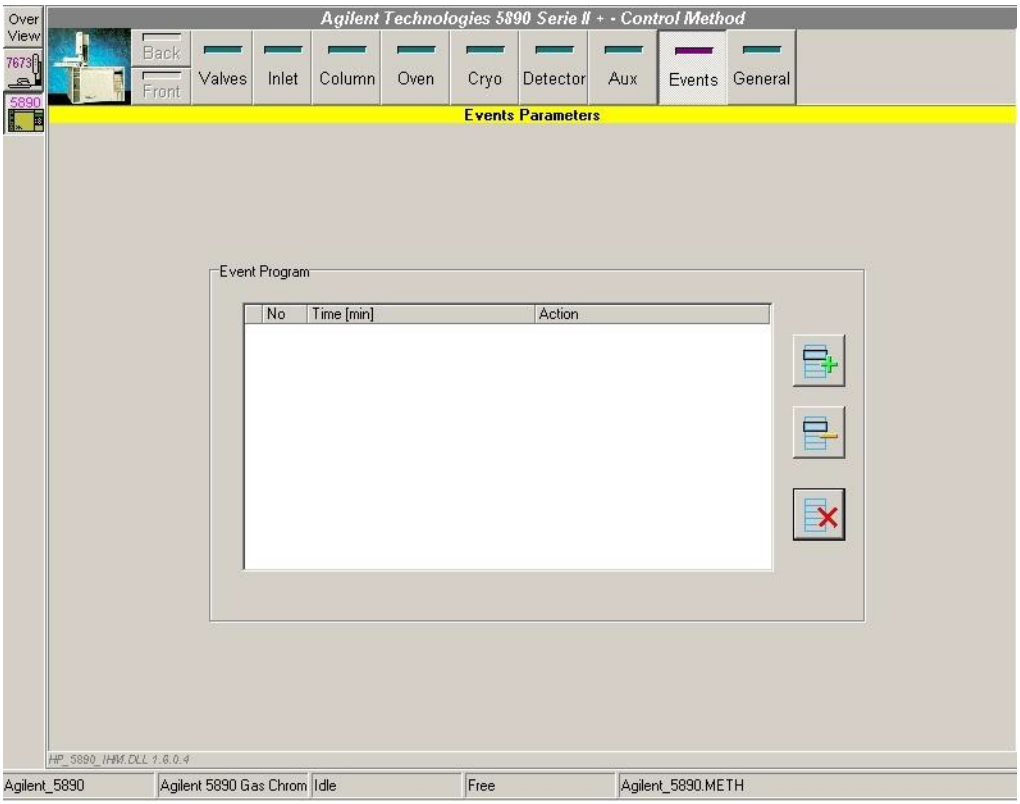
These four auxiliaries allow control of the detector gas flow (make-up gas, carrier gas, and fuel gas), the external sampler gas flow (type ‘purge and trap’ or ‘headspace’), and the optional ‘gas saver’ for split/splitless mode.

Enter the pressure values corresponding to the auxiliaries.

Aux Temperature Parameter Group

Check *On* to turn on the heater and enter the auxiliary temperature.

Events Control



This table allows to program events like valve switching, TCD polarity, signed on/off, etc.

NOTE: If the valve switching is programmed with the event table, it is better to program the initial position of the valve at the end of the analysis.

Use the following buttons to edit the table:

to add a line to the table. to delete a line in the table. to clear the entire table.

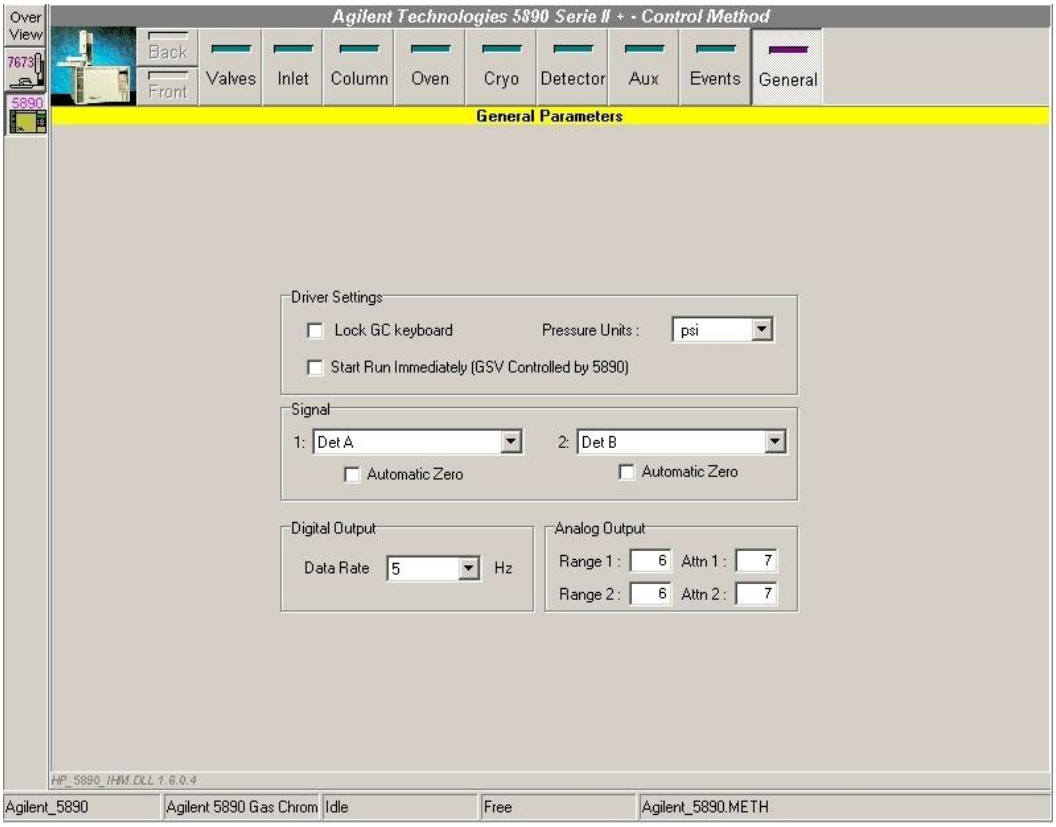
In the column *No*, the number of the line is displayed.

In the column *Time*, enter the time when the action has to be done.

In the column *Action*, select the action to do. The available choices are:

TCD A Low	TCD A Invert Polarity	Valve 3 ON
TCD A High	TCD B Invert Polarity	Valve 3 OFF
TCD B Low	Valve 1 ON	Valve 4 ON
TCD B High	Valve 1 OFF	Valve 4 OFF
Signal Switch ON	Valve 2 ON	
Signal Switch OFF	Valve 2 OFF	

General Control



Driver Settings Parameter Group

Check *Lock GC keyboard* to avoid control parameter modification directly on the chromatograph. The START and STOP keys are operational even when this option is checked.

Check *Start run immediately* to launch an analysis as soon as the GC is ready (in the case of GSV gas sampling valve) without starting it manually.

In the *Pressure Units* area, use the scrolling list to choose the units. The available choices are: psi, bar, kPa.

NOTE: This setting is used for displaying and entering the pressures in the control method subsections described earlier.

Signal Parameter Group

In the field *1* and/or *2*, choose the appropriate signal with the scrolling lists. The available choices are:

Det A	Det B- Comp1	Inlet B Temp
Det B	Det A-Comp 2	Det A Temp
Det A-	Det B- Comp 2	Det B Temp
Det B	Oven Temp	Flow A
Det B-	Comp 1	Flow B
Det A	Comp 2	Test Plot
Det A-Comp 1	Inlet A Temp	

Check *Automatic Zero* (for channel 1 and/or 2) to take into account the background noise and subtract this value from the signal.

Digital Output Parameter Group

In the *Date Rate* field, select the acquisition frequency. The available choices are: *1.25Hz*, *2.5Hz*, *5Hz*, *10Hz* and *20Hz*.

Analog Output Parameter Group

In the *Range* and *Attn* fields, enter the range and attenuation values. These output parameters are valid for analog acquisition. The values depend on the detector installed.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

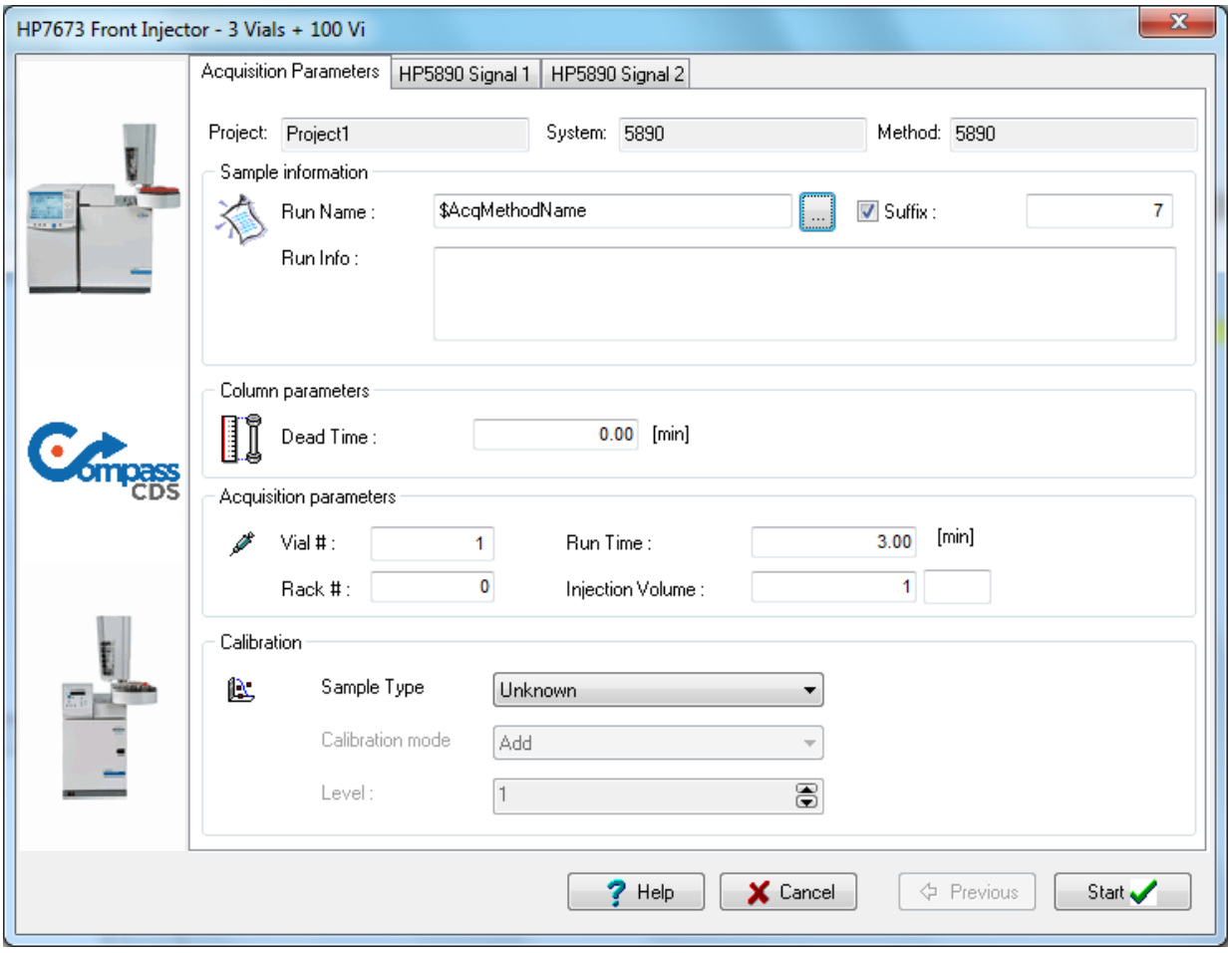
Quick Start (Single Acquisition)

1. Press the button.

   In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

2. Press the OK button.

   The following screen is displayed:



In the *Acquisition parameters* tab, required fields like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

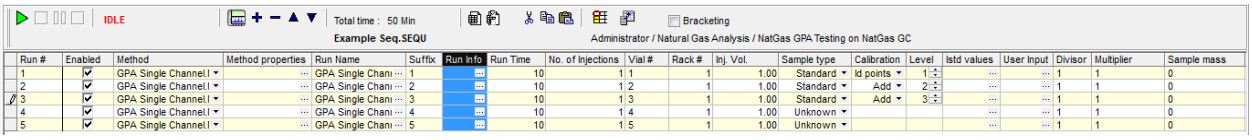
Other parameters associated with each acquisition channel can be entered in the *Channel X* tab.

Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data System User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

2. The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS Chromatography Data System User Guide).



Run #	Enabled	Method	Method properties	Run Name	Suffix	Run Info	Run Time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type	Calibration	Level	Istd values	User Input	Divisor	Multiplier	Sample mass
1	☑	GPA Single Channel.I	...	GPA Single Chan	1	...	10	1	1	1	1.00	Standard	Id points	1	...	...	1	1	0
2	☑	GPA Single Channel.I	...	GPA Single Chan	2	...	10	1	2	1	1.00	Standard	Add	2	...	...	1	1	0
3	☑	GPA Single Channel.I	...	GPA Single Chan	3	...	10	1	3	1	1.00	Standard	Add	3	...	...	1	1	0
4	☑	GPA Single Channel.I	...	GPA Single Chan	4	...	10	1	4	1	1.00	Unknown			...	...	1	1	0
5	☑	GPA Single Channel.I	...	GPA Single Chan	5	...	10	1	5	1	1.00	Unknown			...	...	1	1	0

The Method Name, the Run Name, the Run ID, and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS Chromatography Data System User Guide.

NOTE: The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4 and 5. These values represent the number of tenths of the syringe volume. For example if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 tenths of 10 µL=3 µL. A physical turret option called *Nanoliter* allows the injection of smaller volume (refer to the Agilent manual to learn more about this option). Refer to the Appendix (*Injection Volumes* section) to see the correspondence between the programmed levels and the real injected volumes.

Running Acquisition Status

Viewing a Running Acquisition

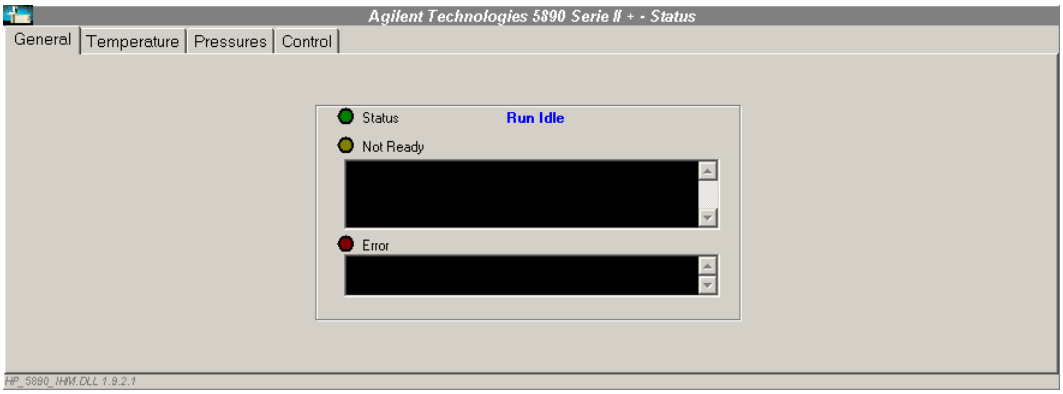
To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Agilent 5890 Gas Chromatograph

Click on the

button corresponding to the Agilent Technologies 5890 Gas Chromatograph driver and the Agilent Technologies 5890 Gas Chromatograph status screen will appear. It contains three sub-sections: *General*, *Temperatures* and *Control.* Depending on the system configuration, a *Pressures* sub-section can be displayed if an EPC or a pressure auxiliary option has been configured. Click on the required sub-section to display the corresponding screen.

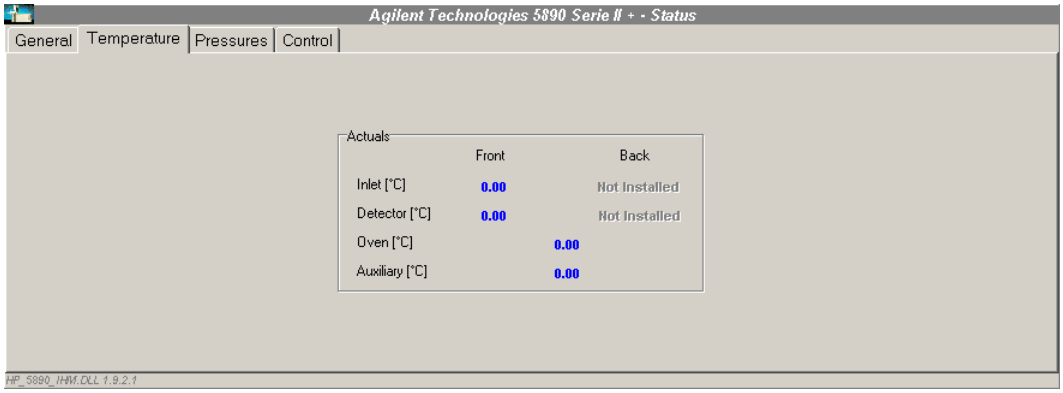
General Window



This is a read-only window.

Information about the instrument status is displayed: Faults, not ready parameters, etc.

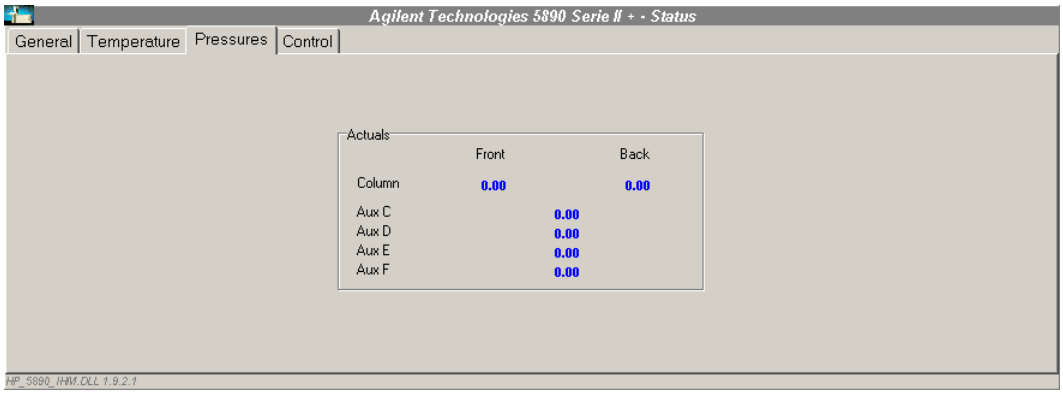
Temperatures Window



This is a read-only window.

The temperatures of the detector(s), inlet(s), oven and auxiliary are displayed.

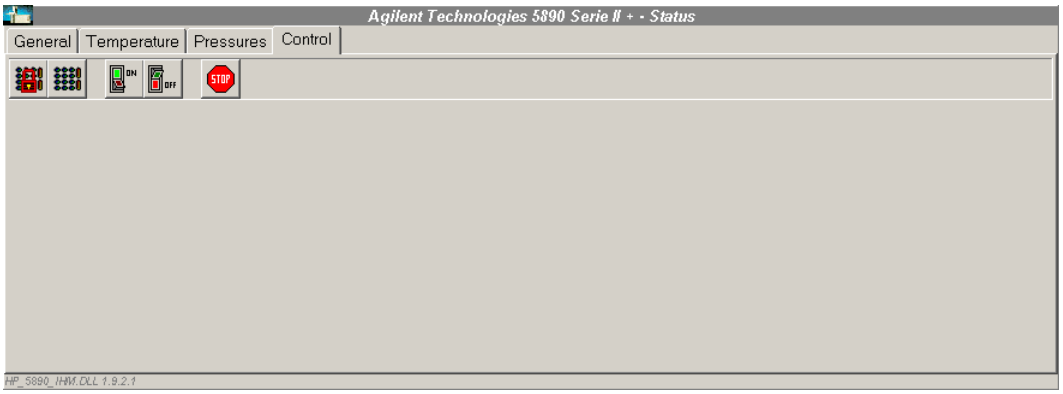
Pressures Window



This is a read-only window.

The pressure in the column(s) and in the auxiliary(ies) is displayed.

Control Window



This window allows direct control of the 5890 GC. The button locks the chromatograph keyboard.

unlocks the chromatograph keyboard.

turns on the 5890 GC

turns off the 5890 GC.

stops the chromatograph.

NOTE: All the direct control buttons are deactivated during a run.

Appendix

Injection Volumes

The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4 and 5. These values represent the number of tenths of the syringe volume. For example if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 tenths of 10 µL = 3 µL. A physical turret option called Nanoliter allows the injection of smaller volume (refer to the Agilent manual to learn more about this option). The following table gives the injected volumes according to the value entered in the Acquisition sub-method part.

Nanoliter Option	Off		On	
	Entered Value	Injected Volume	Entered Value	Injected Volume
5 µL Syringe	1	0.5	1	0.1
	2	1.0	2	0.5
	3	1.5	3	1.0
	4	2.0	4	1.5
	5	2.5	5	2.0
10 µL Syringe	1	1.0	1	0.2
	2	2.0	2	1.0
	3	3.0	3	2.0
	4	4.0	4	3.0
	5	5.0	5	4.0
25 µL Syringe	1	2.5	1	0.5
	2	5.0	2	2.5
	3	7.5	3	5.0
	4	10.0	4	7.5
	5	12.5	5	10.0
50 µL Syringe	1	5.0	1	1.0
	2	10.0	2	5.0
	3	15.0	3	10.0
	4	20.0	4	15.0
	5	25.0	5	20.0
100 µL Syringe	1	10.0	1	2.0
	2	20.0	2	10.0
	3	30.0	3	20.0
	4	40.0	4	30.0
	5	50.0	5	40.0

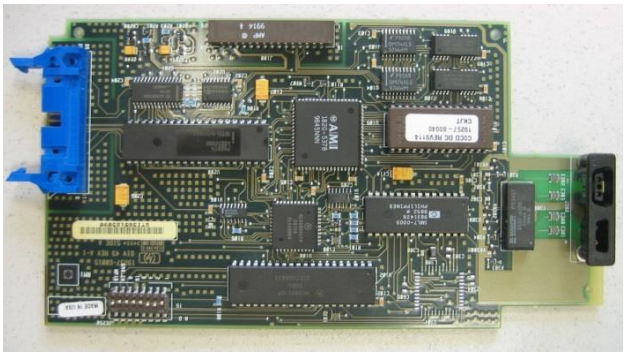
Configuring a 5890 GC to CompassCDS

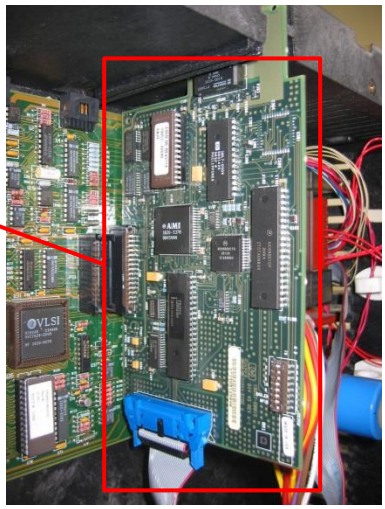
Every 5890 that will be controlled by CompassCDS must have the HPIB/RS232 communication kit installed.

If the GC was formerly controlled by Agilent Chemstation, it will have the HPIB/RS232 communication kit already installed.

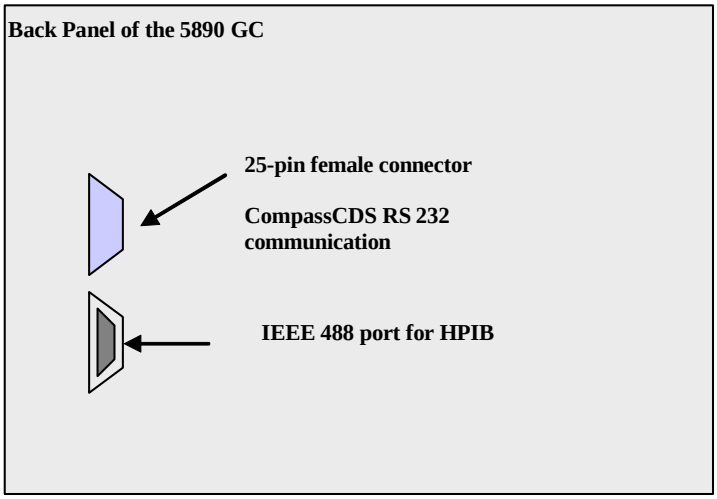
This kit contains three parts:

- a board on the right-hand side of the GC. To access this board, remove the right panel of the GC (tightened by 4 screws) as shown below :





- Connectors on the back of the GC : The back of the GC has 2 connectors : an IEEE 488 connector used by Agilent Chemstation for HPIB communication, and a 25-pin RS 232 female connector used for CompassCDS RS 232 control.



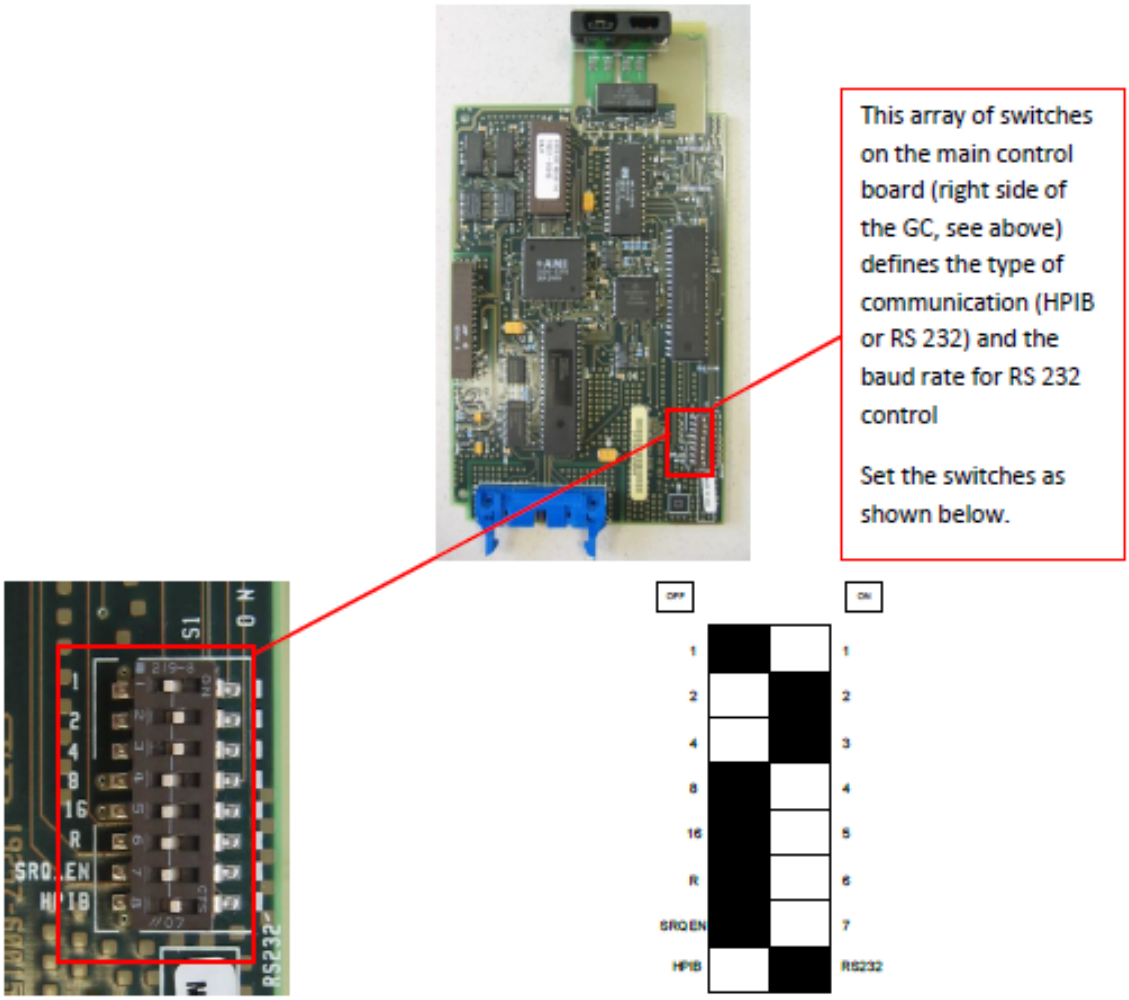
- Connectors on the top of the GC: Be sure to connect the 82167-60002 Agilent part number cable in the “Instrument Network Out/In” plugs (this connection is necessary for [CompassCDS starting when the GC starts).

Setting and Configuration

When connected to Chemstation, the GC is set up for communication with IEEE488 (HPIB) interface. The RS232 baud rate is by default not set on the GC.

To set it to the proper value for CompassCDS (9600 bauds), do the following steps:

Step 1: Power-off the GC and configure the switches on the control board as shown below



Step 2: Verify the baud rate on the GC

Power on the GC again, and hold the [**clear**] key pressed during GC initialization. The message « **User Test Sel 0..7** » will appear.

Press [**4**] : the GC will display « **RS232 baud = 9600** ».

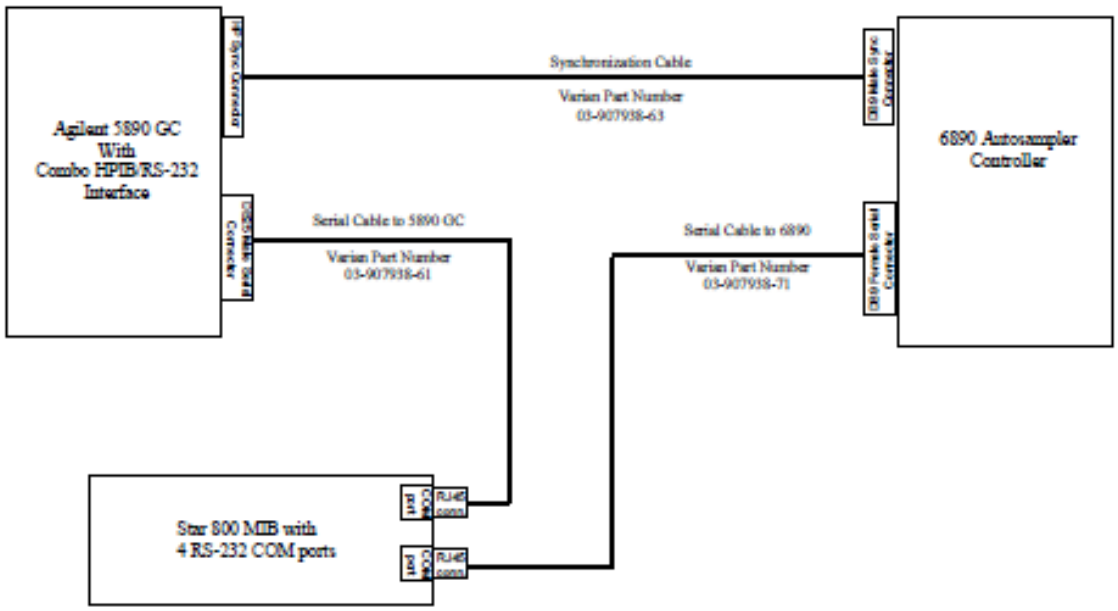
If the GC does not display this message, verify the configuration of the switches on the board (see above)

Wiring Connections between CompassCDS and the 5890 GC with Autosampler

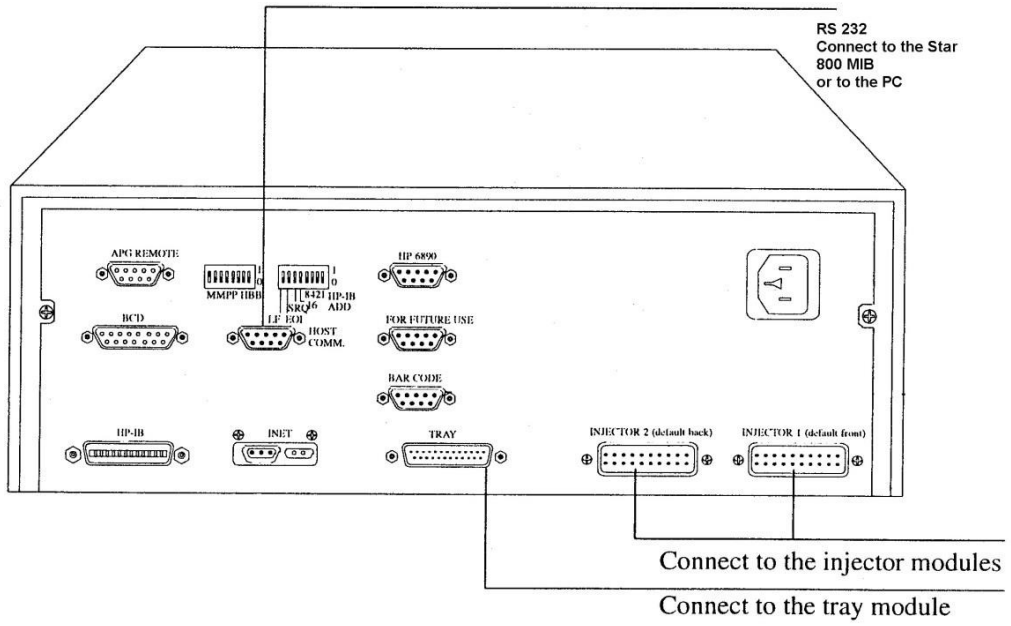
Depending on which autosampler controller is used with the 5890 GC, the cables between the 5890 GC and the autosampler controller and the cables between the autosampler controller and the MIB-interface (or the PC) are different.

All the needed information is shown in the following drawings.

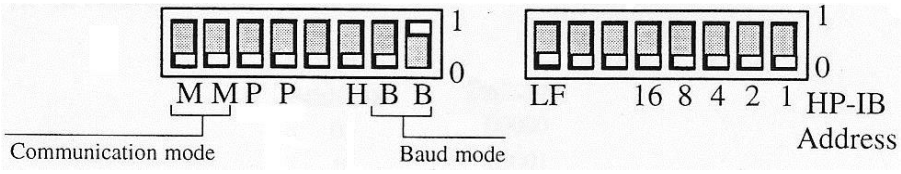
Agilent 5890 GC with 6890 Autosampler Controller Connected to MIB-interface COM ports



With this type of controller, only the communication switches must be set to define RS232 as communication mode and 9600 as baud rate.

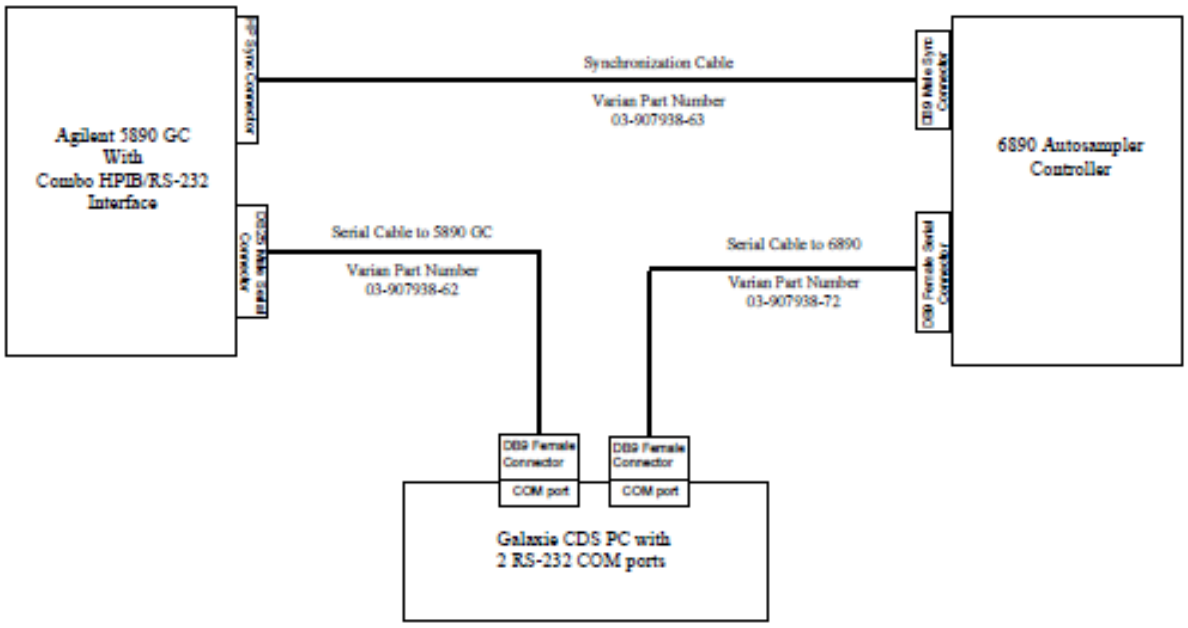


Make sure that the switches on the back of the controller are set up as shown.

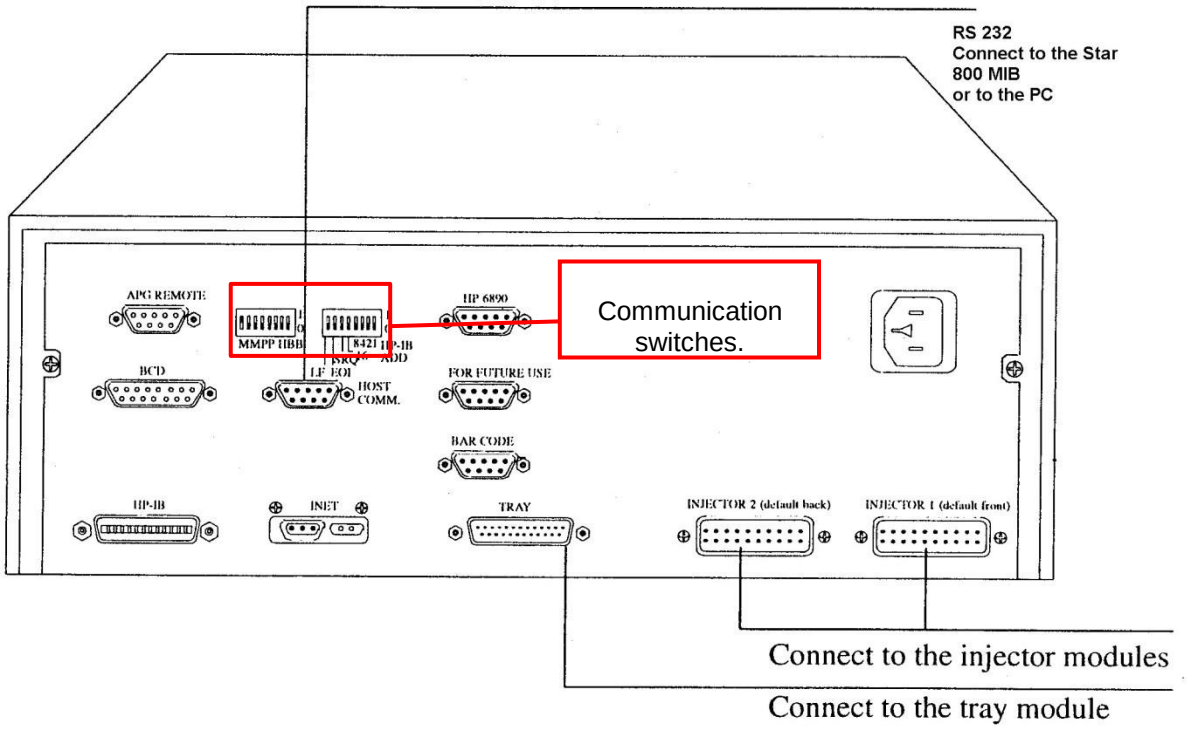


The communication cable from the controller to the MIB-interface (or the PC) must be plugged in the "**HOST COMM**" connector and the synchronization cable from the controller to the GC must be plugged in the "**Remote APG**" connector.

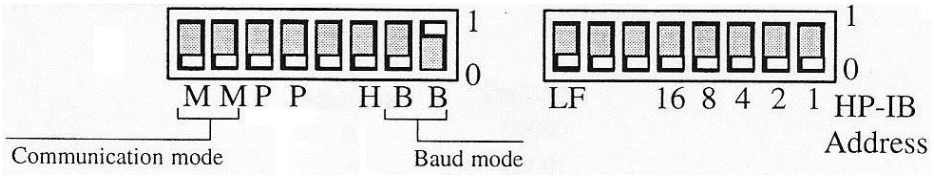
Agilent 5890 GC with 6890 Autosampler Controller Connected to PC COM ports



With this type of controller, only the communication switches must be set to define RS232 as communication mode and 9600 as baud rate.

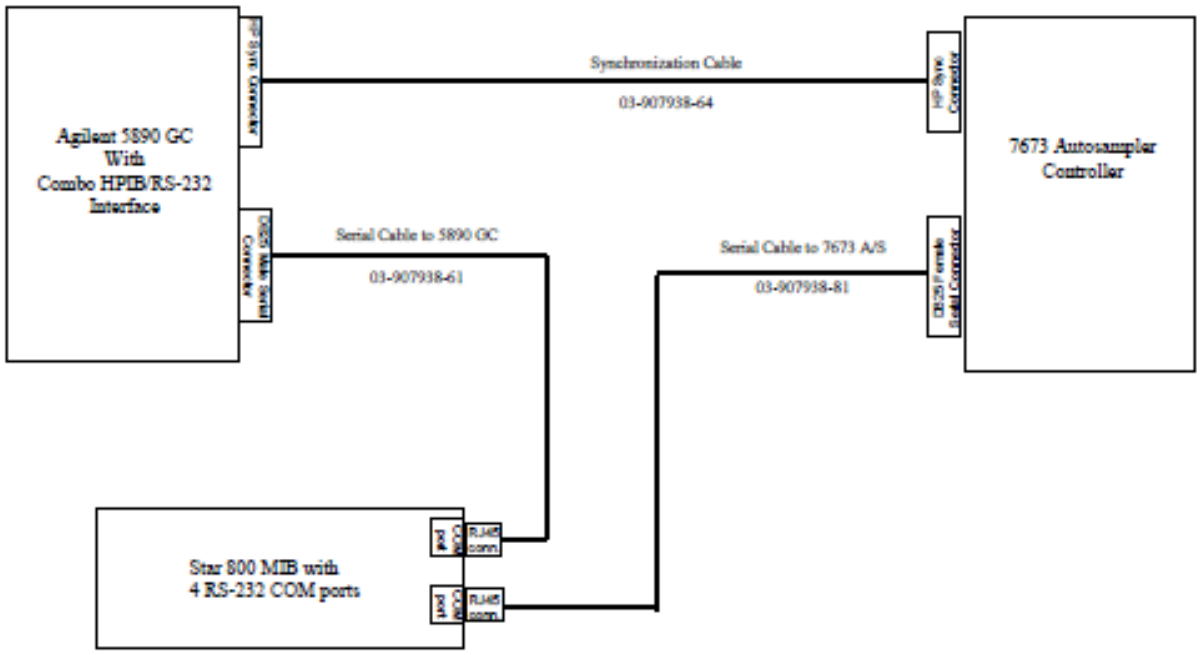


Make sure that the switches on the back of the controller are set up as shown.



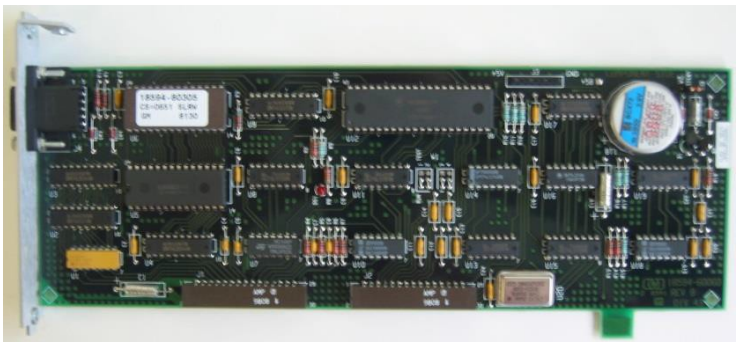
The communication cable from the controller to the MIB-interface (or the PC) must be plugged in the "**HOST COMM**" connector and the synchronization cable from the controller to the GC must be plugged in the "**Remote APG**" connector.

Agilent 5890 GC with 7673 Autosampler Controller Connected to MIB-interface COM ports



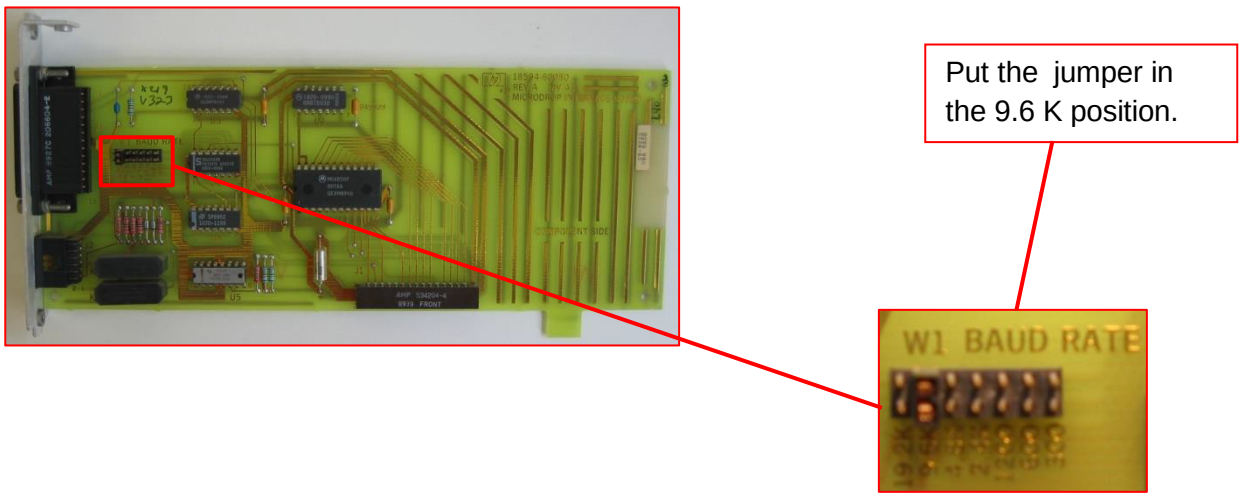
The autosampler controller mother card (*Controller* position in the 7673 controller) must be the one without GPIB connector on it to be able to communicate with CompassCDS (board reference HP_18594-60060). If not (for example the HP_18594-60110 card with a GPIB connector on it), you will not be able to communicate with the autosampler.

NOTE: The synchronization cable is no longer needed since version 1.11.1.6 of the 7673 autosampler. If upgrading the driver of the 5890 to a version greater or equal to the 1.14.1.1, remove this cable.

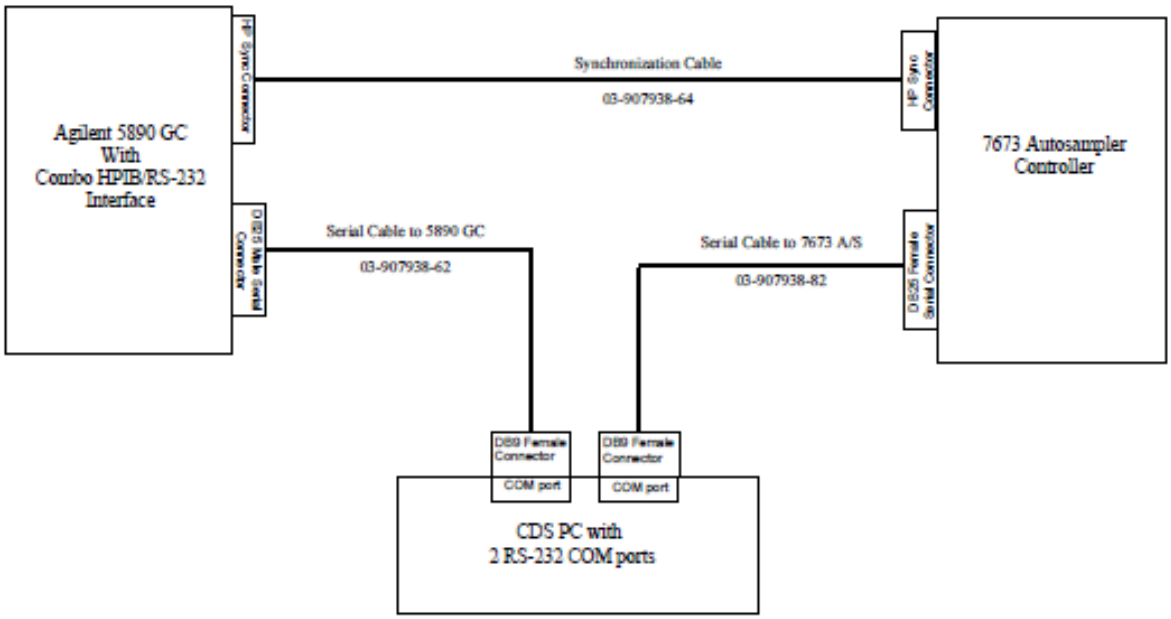


Controller board without GPIB (ref: HP_18594-60060)

Furthermore, the jumper on the *Communication* board of the autosampler must in the position 9.6K as shown below.

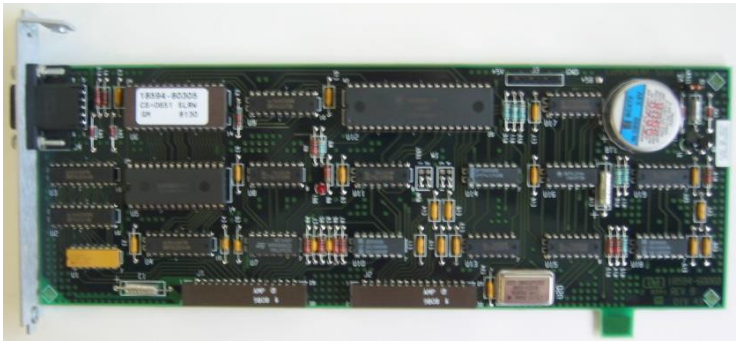


Agilent 5890 GC with 7673 Autosampler Controller Connected to PC COM ports



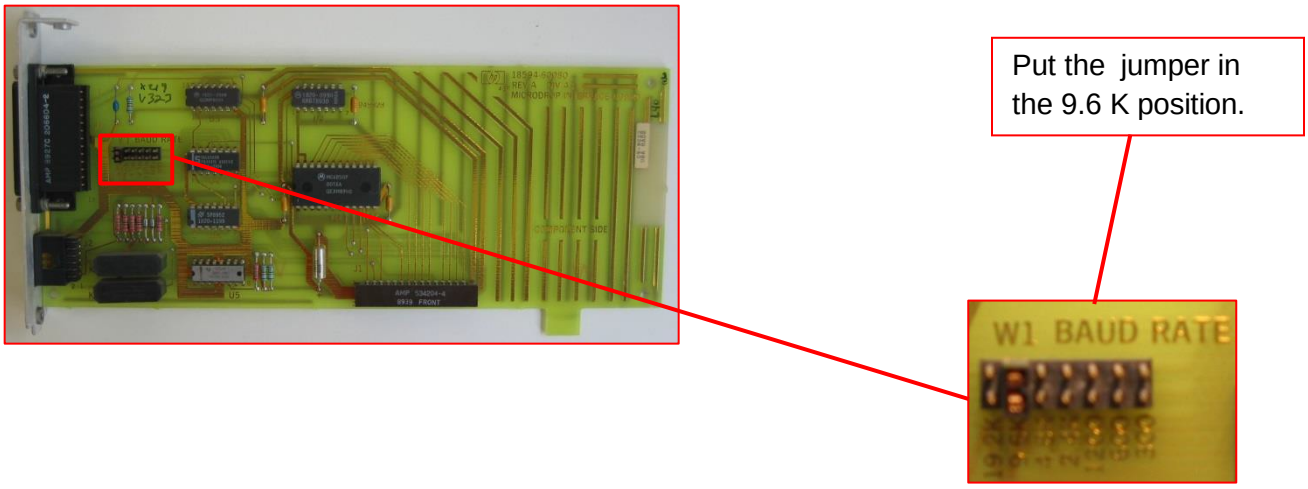
The autosampler controller mother card (*Controller* position in the 7673 controller) must be the one without GPIB connector on it to be able to communicate with CompassCDS (board reference HP_18594-60060). If not (for example the HP_18594-60110 card with a GPIB connector on it), you will not be able to communicate with the autosampler.

NOTE: The synchronization cable is no longer needed since version 1.11.1.6 of the 7673 autosampler. If upgrading the driver of the 5890 to a version greater or equal to the 1.14.1.1, then, just remove this cable.



Controller board without GPIB (ref :HP_18594-60060)

Furthermore the jumper on the *Communication* board of the autosampler must in the position 9.6K as shown below.



Agilent 5890 GC Control Driver Release Notes

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501584
Revision C

Introduction of the driver (4.0.0)

The Agilent 5890 GC CompassCDS control driver software needs CompassCDS version 3.0.1 or above (CompassCDS version 2.0 is not supported).

The Agilent 5890 GC can be controlled by CompassCDS software when equipped with the HPIB & RS232 communication board, and the 7673 AS when connected to the PC COM port or the GPIB port of a STAR 800 & 850 MIB.

Supported configurations

- Inlets:
  Split/splitless capillary inlet (S/SL)
  Temperature-programmable cool on-column inlet (PCOC)
- Detectors:
  Flame ionization detector (FID)
  Thermal conductivity detector (TCD)
  Electron capture detector (ECD)
  Nitrogen Phosphorous detector (NPD)
  Flame Photometric Detector (FPD)
- Autosampler: Automatic liquid sampler (ALS) type 7673 (G1513A) including the 100 vials tray (18596A) and the controller module (G1512A)
- The Oven Cryogenic coolant is controlled
- PCM (Pressure Control Module) is controlled
- Multi injector, multi detector: CompassCDS can control any 2 autosampler, 2 Inlet, 2 detector configuration as long as the configuration consists of the elements described above
- Valves. Four valves can be controlled.
- One auxiliary heater can be controlled.
- Four auxiliary EPCs can be controlled
- Run time events

Known issues

- The inlet temperature program of the method is still applied when changing from Programmable inlet or Oven track inlet to Isothermal inlet. The workaround is to set all ramp values to 0.
- When the 5890 has a version greater or equal to 1.14.1.1, using an Agilent 7673 Autosampler connected using serial communication, and using a driver version greater or equal to 1.11.1.6, it can occur that the injection is done, but the Ready signal is not sent back to CompassCDS. Then, no data point is displayed on the acquisition view. In this case, remove the synchronization cable.

Agilent 7673 Autosampler Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501580
Revision C

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the Driver 3
    Configuring the Agilent 7673 Autosampler 3
Building a Method 5
  Creating a New Method 5
  Control Method Section for the Agilent 7673 Autosampler 7
Starting and Viewing an Acquisition 9
  Quick Start and Sequence 9
    Quick Start (Single Acquisition) 9
    Sequence 10
  Running Acquisition Status 11
    Viewing a Running Acquisition 11
    Status of the Agilent 7673 Autosampler 11
    Overview Window 11

Introduction

This document describes the configuration of the Agilent Technologies 7673 Autosampler driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

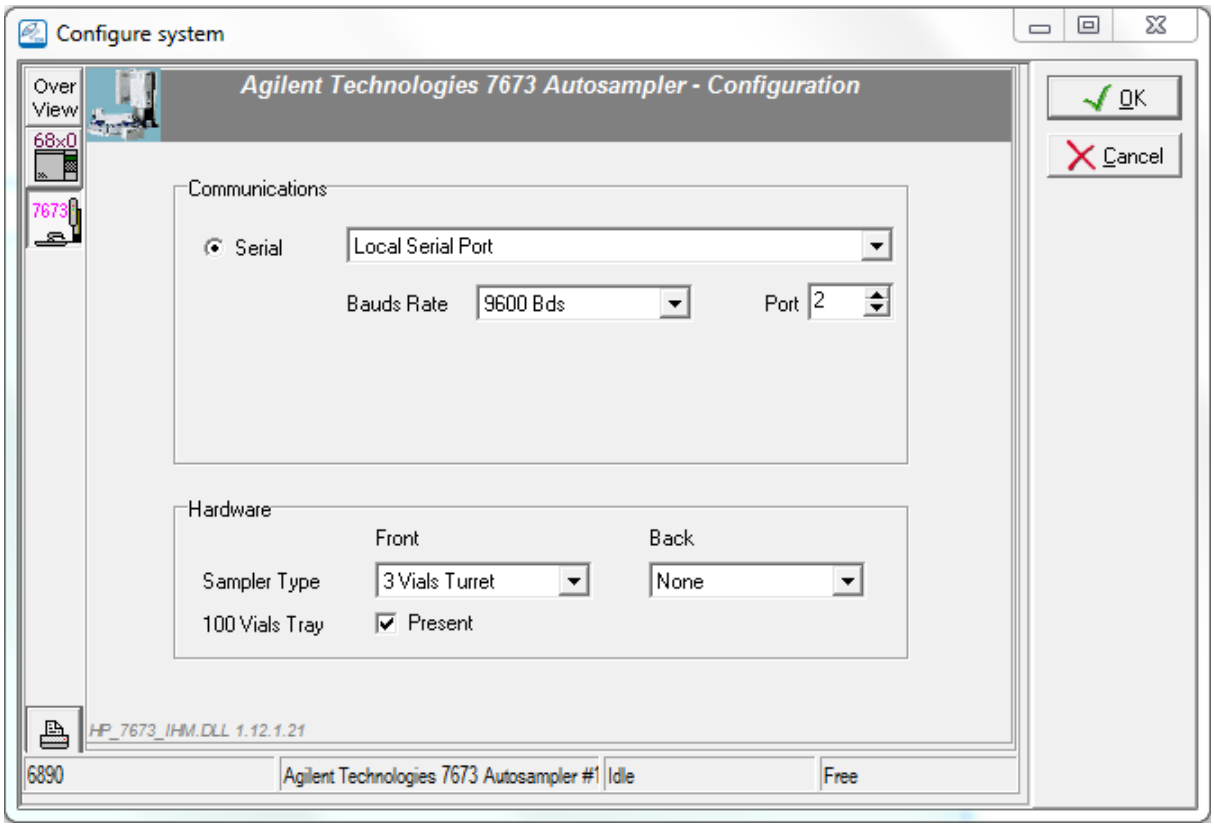
Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Agilent 7673 Autosampler

Click on the

button corresponding to the Agilent 7673 Autosampler driver and the configuration screen appears:



Communication Parameter Group

Serial:

Choose Serial if the 7673 controller uses a serial communication. Select *Local Serial Port* if the autosampler is directly connected to the PC or the name of the STAR 800 & 850 MIB-interface used to connect the autosampler.

Baud Rate:

Choose 9600 Bds

Port:

Select the PC or STAR 800 & 850 MIB-interface Serial port number on which the autosampler will be connected.

NOTE: If you will use the Serial port installed in the MIB-interface, configure the STAR 800 & 850 MIB-interface before configuring the Agilent Technologies 7673 autosampler.

Hardware Parameter Group

Sampler Type:

Select the Front and Back Sampler Type. The available choices are: None, 3 Vials Turret and 8 Vials Turret.

Check Present If the chromatographic system is equipped with a 100 Vial Tray.

To save the configuration, accept the configuration of the system by clicking on the OK button. Then right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

NOTE: Once the system has been created and correctly configured, it must be associated to one or several projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration.

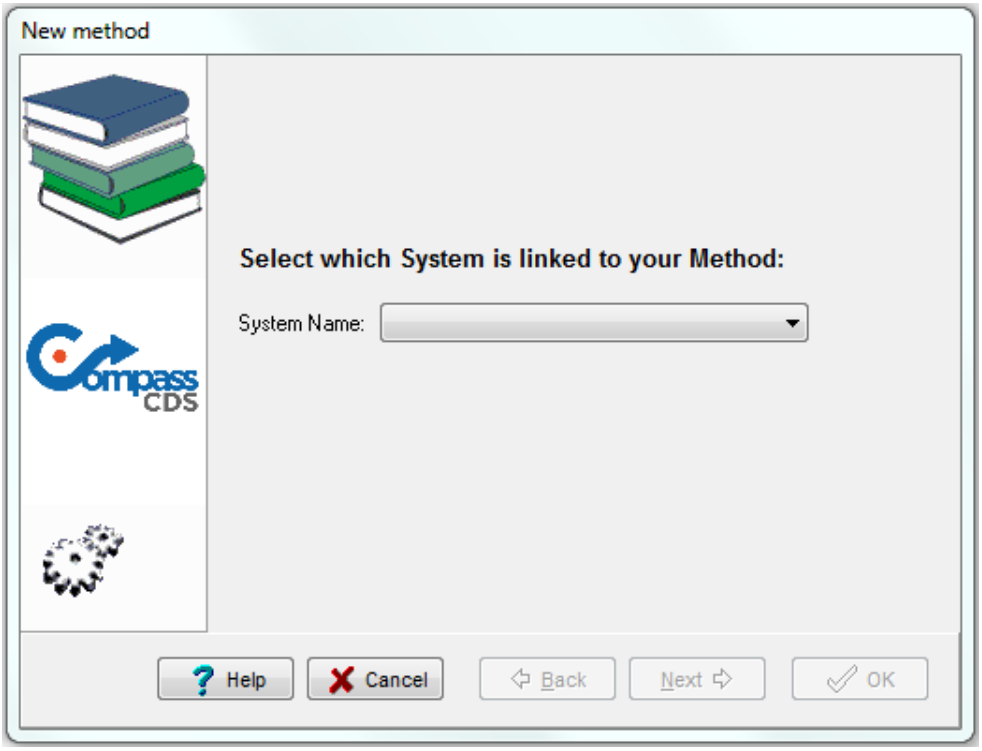
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

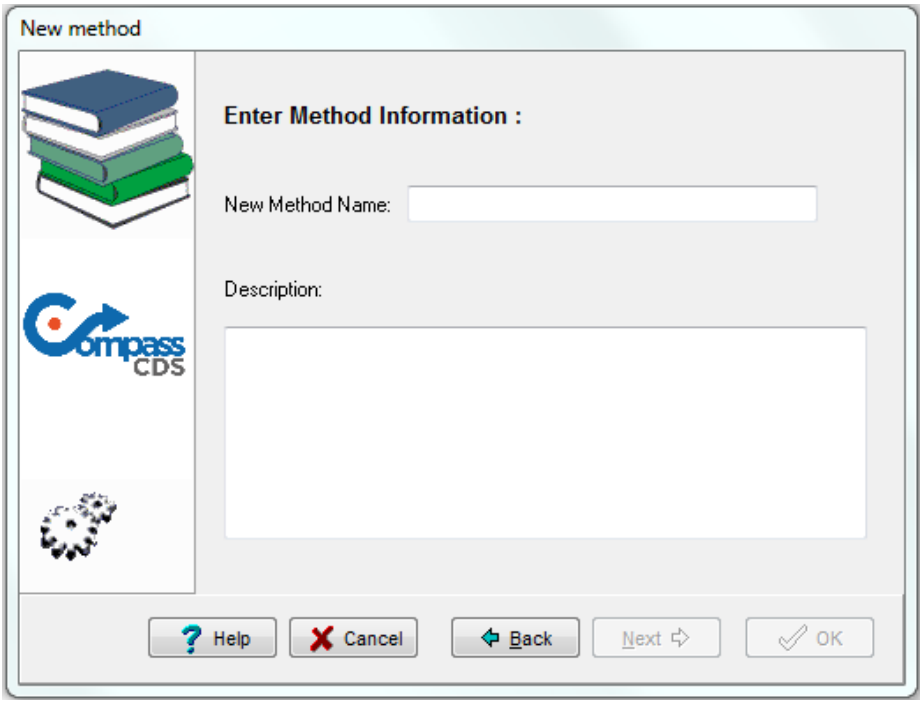
To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS Chromatography Data System main menu.

A wizard guide will appear and provide assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

Once this field is completed, click on the Next button to move to the second step of the method creation:



Enter the *New Method Name* in the first field. In the *Description* field, enter information concerning the method (optional).

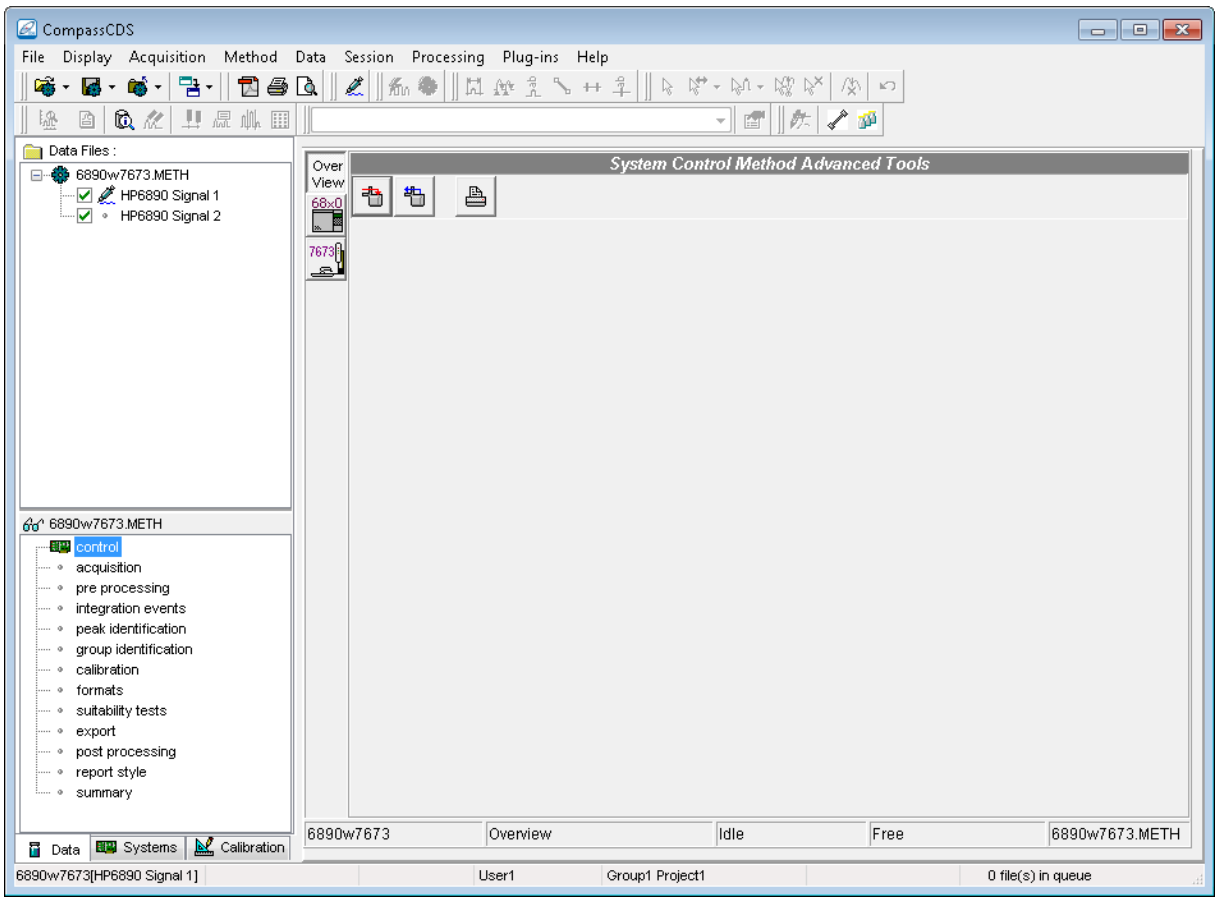
Once these two fields have been completed, click on the *OK* button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

The instrument control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Agilent 7673 Autosampler is detailed. Other parameters such as *Injection Volume*, *Vial* and *Rack* number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, refer to the CompassCDS User Guide.

Control Method Section for the Agilent 7673 Autosampler

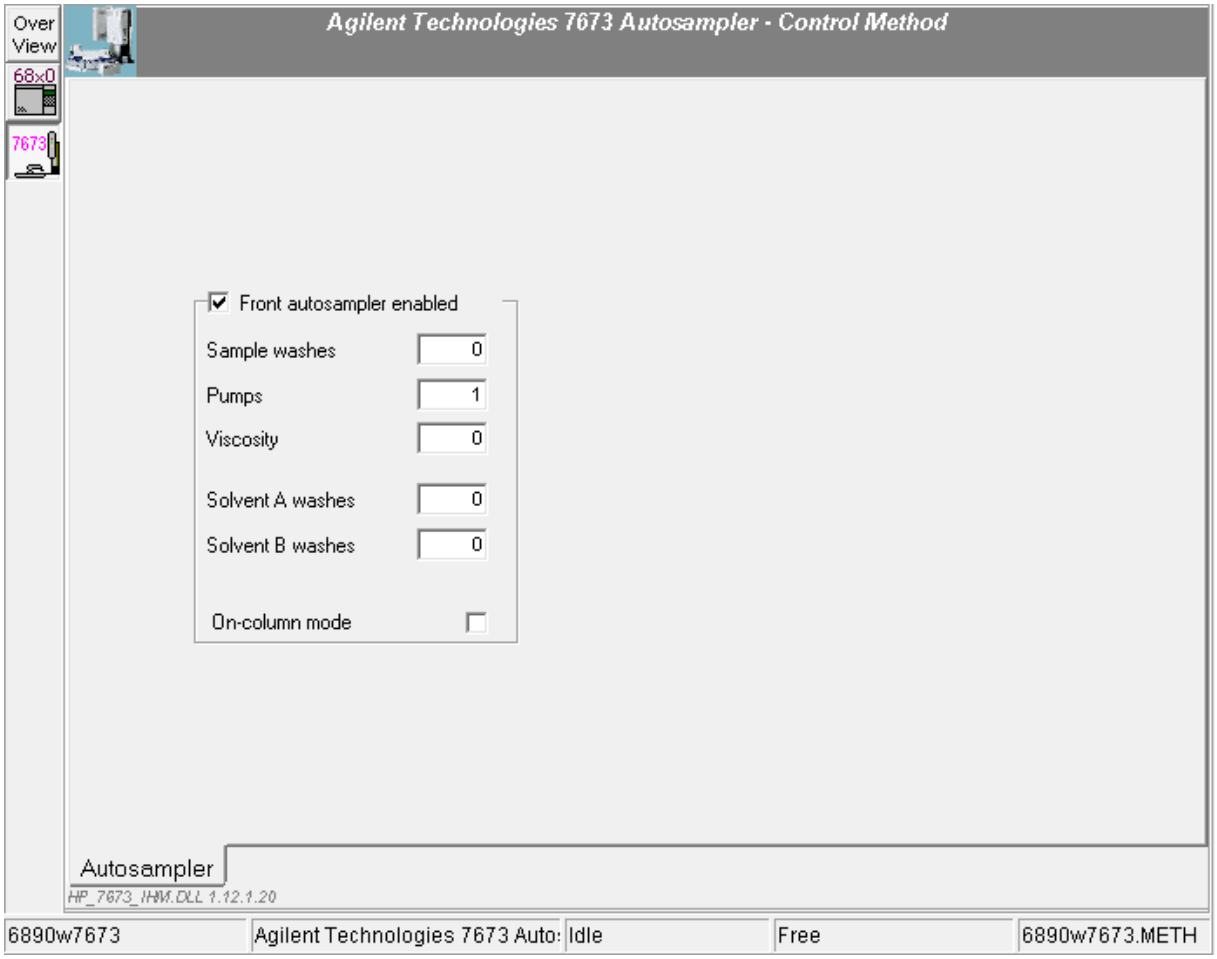
Once the new method is created, select the control section in the lower part of the browser. The following screen appears:



Click on the

button to display the Agilent 7673 Autosampler control method section.

Depending on the system configuration, the displayed window will contain one or two parameter groups. If only a front (or back) autosampler is configured, only the *Use Front* (or *Back*) *Autosampler* parameter group will be displayed. If both autosamplers are configured, the *Use Front Autosampler* and *Use Back Autosampler* parameter groups are displayed.



Check *Use Front (*and/or *Back) Autosampler* to take into account the autosampler parameters.

To inject manually for a short time, in the control section of the method, uncheck *Use Front (*and/or *Back) Autosampler*. Press on the start button of the GC after the manual injection.

In the *Sample Washes* field, enter the number of syringe washes with the sample, before injection.

In the *Pumps* field, enter the number of pumps before the injection (plunger strokes to avoid the formation of bubbles).

In the *Viscosity* field, enter a time (in seconds). During this time, the syringe plunger pauses between the pumping and the injection stroke. For viscous samples, the pause allows the sample to flow into the vacuum created in the syringe.

In the *Solvent Washes A/B*, enter the number of syringe washes with solvent A and/or B. Check the *On column* mode for on column injection.

NOTE: The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4 and 5. These values represent the number of tenths of the syringe volume. For example, if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 tenths of 10 µL = 3 µL. A physical turret option called Nanoliter allows the injection of smaller volume (refer to the Agilent manual to learn more about this option). Refer to the Appendix (Injection Volumes section) to see the correspondence between the programmed levels and the real injected volumes.

Transfer Line: Enter in this field the transfer line temperature.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

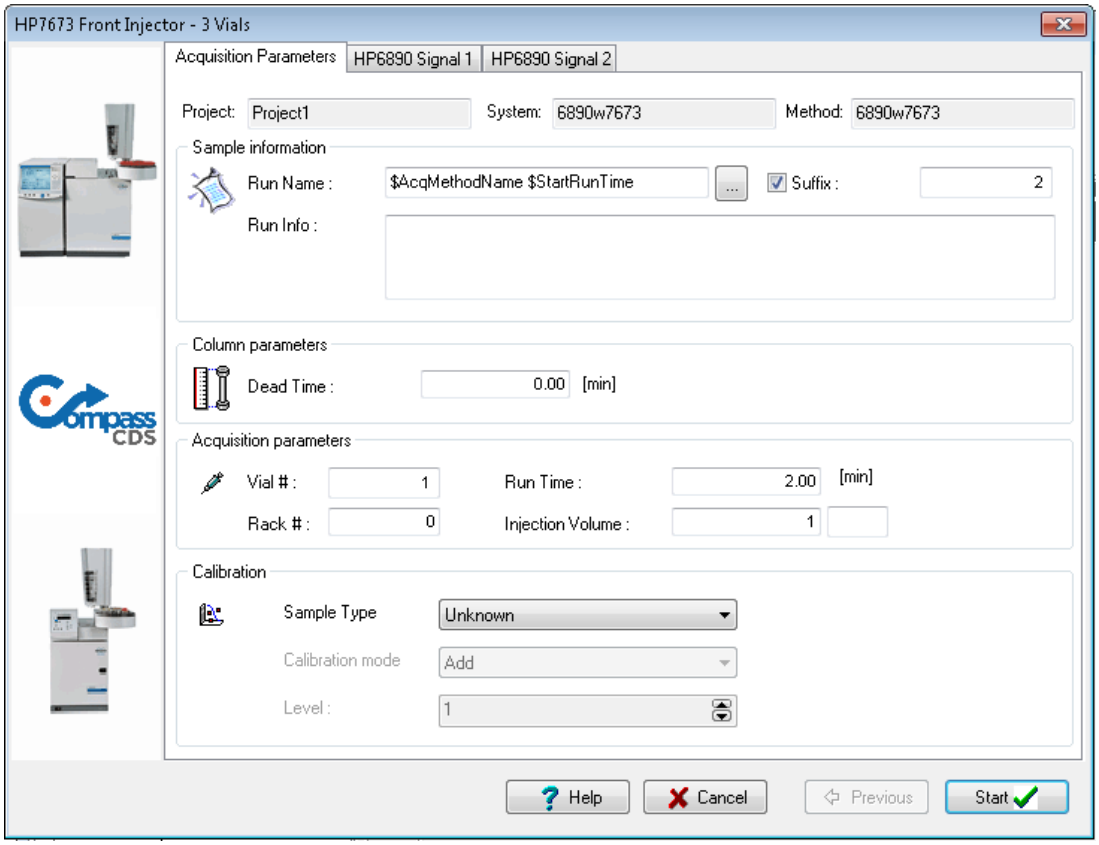
Quick Start (Single Acquisition)

Press the button.

In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

Press the OK button.

The following screen is displayed:



In the *Acquisition parameters* tab, required fields like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the *Channel X* tab.

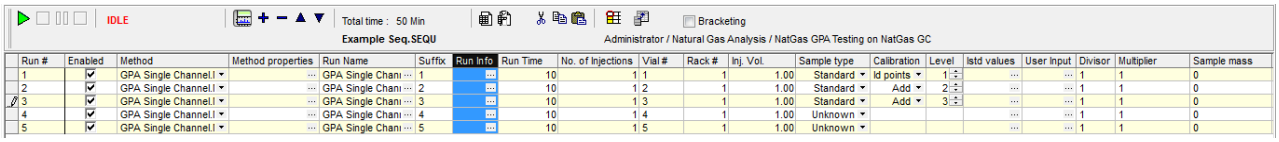
Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data

System User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS User Guide).


IDLE
Total time : 50 Min
Example Seq.SEQU
Bracketing
Administrator / Natural Gas Analysis / NatGas GPA Testing on NatGas GC
Run # | Enabled | Method | Method properties | Run Name | Suffix | Run Info | Run Time | No. of Injections | Vial # | Rack # | Inj. Vol. | Sample type | Calibration | Level | Istd values | User Input | Divisor | Multiplier | Sample mass
1 | GPA Single Channel.I | GPA Single Chani | 1 | 10 | 1 | 1 | 1 | 1.00 | Standard | Id points | 1 | 1 | 1 | 0
2 | GPA Single Channel.I | GPA Single Chani | 2 | 10 | 1 | 2 | 1 | 1.00 | Standard | Add | 2 | 1 | 1 | 0
3 | GPA Single Channel.I | GPA Single Chani | 3 | 10 | 1 | 3 | 1 | 1.00 | Standard | Add | 3 | 1 | 1 | 0
4 | GPA Single Channel.I | GPA Single Chani | 4 | 10 | 1 | 4 | 1 | 1.00 | Unknown | 1 | 1 | 0
5 | GPA Single Channel.I | GPA Single Chani | 5 | 10 | 1 | 5 | 1 | 1.00 | Unknown | 1 | 1 | 0

The *Method Name*, the *Run Name*, the *Run ID,* and the *Acquisition length* must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS User Guide.

NOTE: The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4 and 5. These values represent the number of tenth of the syringe volume. For example, if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 10^{nth}= 3 µL. A physical turret option called *Nanoliter* allows the injection of smaller volume (refer to the Agilent manual to know more about this option). Refer to the Appendix (*Injection Volumes* section) to see the correspondence between the programmed levels and the real injected volumes.

Running Acquisition Status

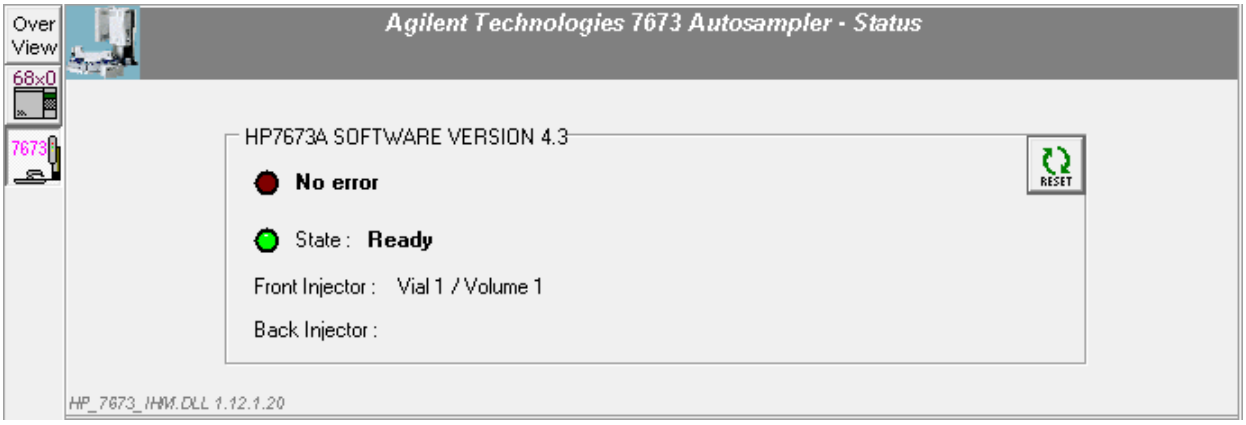
Viewing a Running Acquisition

To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Agilent 7673 Autosampler

Click on the

button corresponding to the Agilent 7673 Autosampler driver and the Agilent Technologies 7673 Autosampler status screen will appear.



This is a read-only window.

The screen displays the state of the autosampler.

Information about the *Vial* and the *Volume* for the *Front* and *Back Injectors* are displayed.

NOTE: When the autosampler communicates with Compass, the firmware version is displayed above the *Communication Error* LED.

NOTE: If you are connecting by GPIB, a tray is configuring on your Autosampler and you stop the acquisition in prerun, the tray will continue its work (put vials in front and rear towel, then put back vials on the tray). If you are connecting by Serial communication, a tray is configuring on your Autosampler and you stop the acquisition in waiting for injection, the tray will stop its work immediately. If you launch the same method again the tray will begin by putting back vials on the tray. If you launch another method you should first manually put back vials on the tray otherwise you can have an ERROR TRAY issue.

Overview Window

Click on the

button: for this driver, nothing is displayed.

Agilent 7694 Headspace Autosampler Control Driver
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501582
Revision C

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the Driver 3
    Configuring the Agilent 7694 Headspace Autosampler 3
Building a Method 5
  Creating a New Method 5
  Control Method Section for the Agilent 7694 Headspace Autosampler 7
    Parameters Control 8
    Sampling Control 9
    Temperature Control 10
    Timing Control 11
Starting and Viewing an Acquisition 12
  Quick Start and Sequence 12
    Quick Start (Single Acquisition) 12
    Sequence 13
  Running Acquisition Status 13
    Viewing a Running Acquisition 13
    Status of the Agilent 7694 Headspace Autosampler 13
    Headspace Status 14
    Sampler Status 14
    Overview Window 14

Introduction

This document describes the configuration of the Agilent Technologies 7694 Headspace Autosampler driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

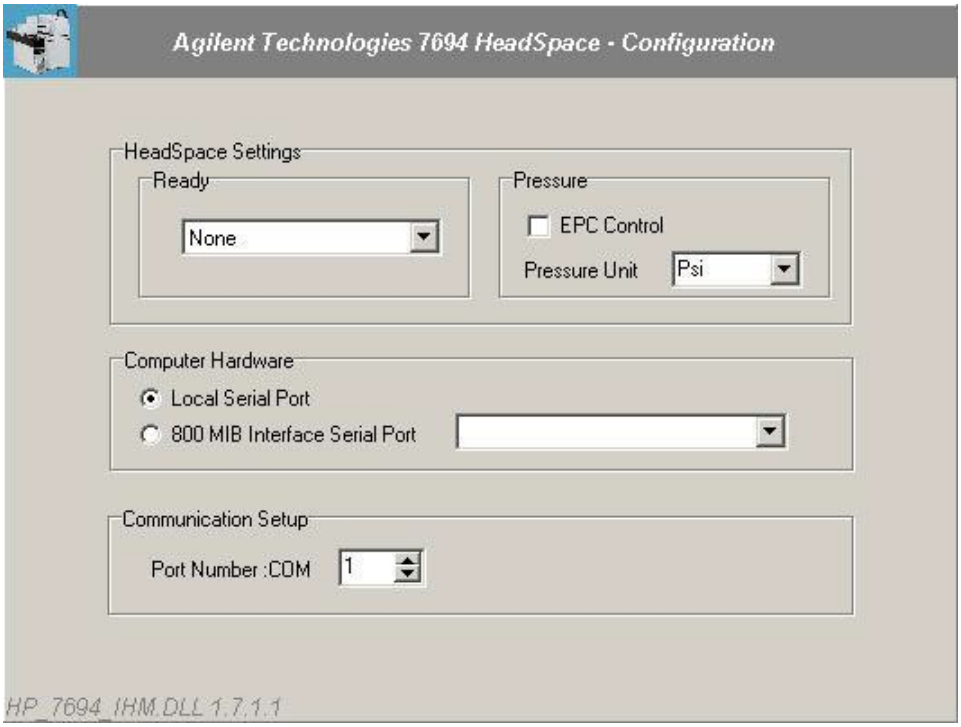
Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Agilent 7694 Headspace Autosampler

Click on the

button corresponding to the Agilent 7694 Headspace Autosampler driver and the configuration screen appears:



Headspace settings Parameter Group

Ready:

Select in the scrolling list the behavior of the autosampler when it is ready to inject. If None is selected the autosampler will always inject when ready. If Wait is selected, the autosampler will wait

for the GC to be ready to inject. Finally, if Abort is selected the autosampler will abort the injection if the GC is not ready.

EPC Control:

Check the box if the autosampler is equipped with an electronic pressure control.

Pressure Unit:

Select in the dropdown list the pressure unit that will be displayed in the status. Three choices are available: Psi, Kpa and Bar.

Computer Hardware settings Parameter Group

Local Serial Port:

Select this option if the chromatograph is directly connected to the PC.

STAR 800 & 850 MIB-Interface Serial Port:

Select this option and then the name of the STAR 800 & 850 MIB -interface used to connect to the chromatograph.

NOTE: If you will be using the serial port installed in the STAR 800 & 850 MIB -interface, configure the MIB-interface before configuring the Agilent Technologies 7694 Headspace AutoSampler driver.

Communication Setup Parameter Group

Port Number: COM

Select the PC or STAR 800 & 850 MIB-interface Serial port number on which the autosampler will be connected.

NOTE: Once the system has been created and correctly configured, it must be associated to one or more projects to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration.

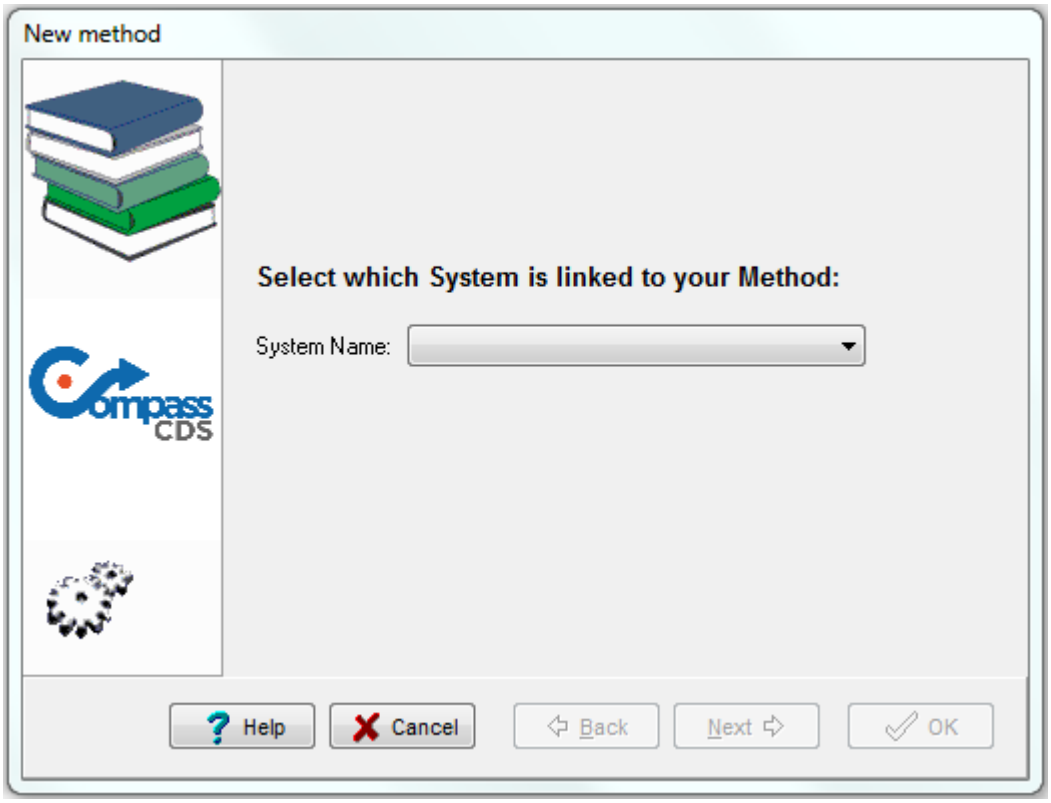
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

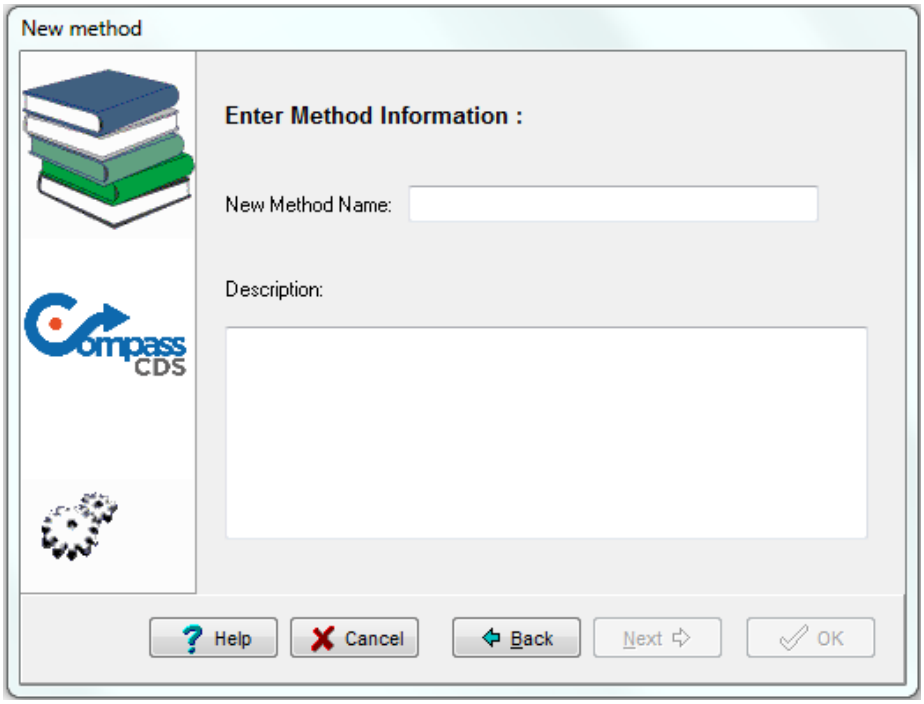
To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS Chromatography Data System main menu.

A wizard guide will appear and provide assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

Once this field is completed, click on the Next button to move to the second step of the method creation:



Enter the *New Method Name* in the first field. In the *Description* field, enter information concerning the method (optional).

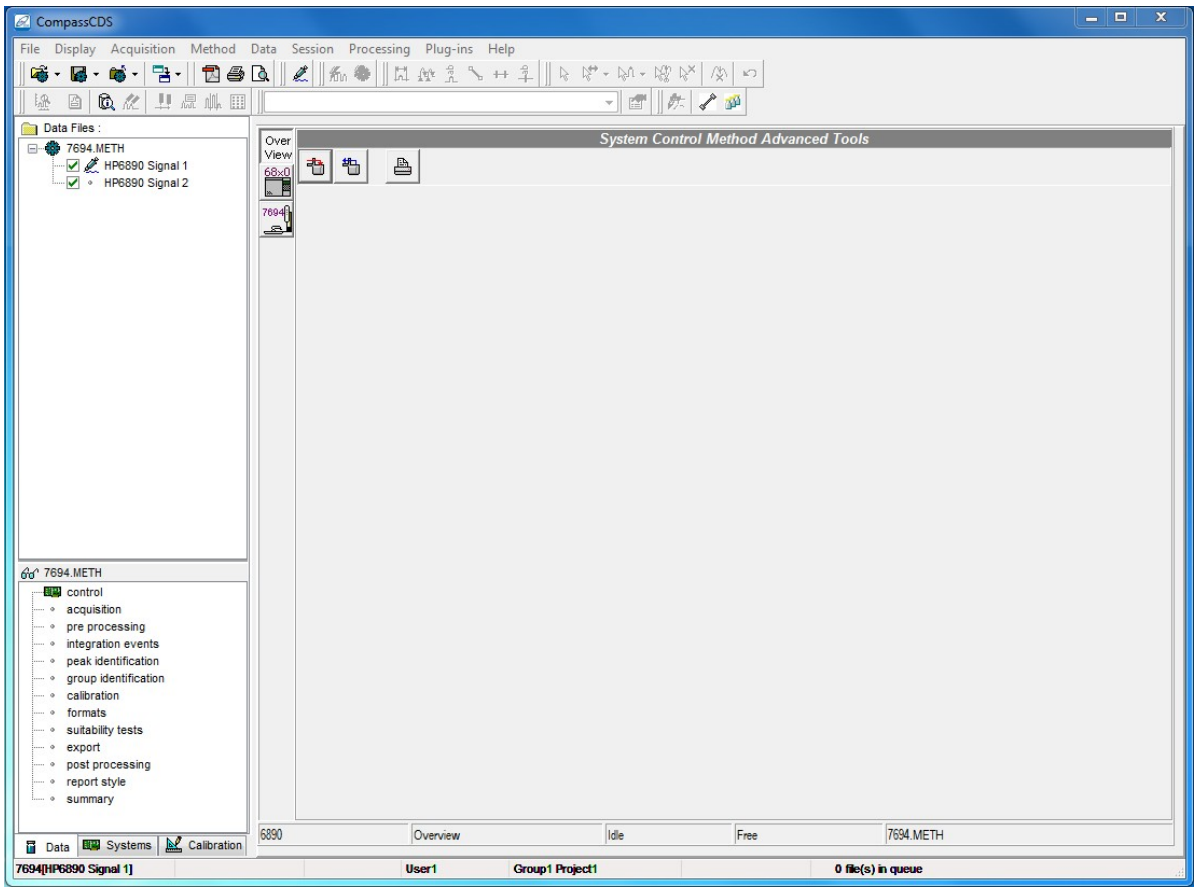
Once these two fields have been completed, click on the *OK* button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

The instrument control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Agilent 7694 Headspace Autosampler is detailed. Other parameters such as *Injection Volume*, *Vial* and *Rack* number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to the CompassCDS User Guide.

Control Method Section for the Agilent 7694 Headspace Autosampler

Once the new method is created, select the control section in the lower part of the browser. The following screen appears:



Press the button to display the System Control Method Advanced Tools window:

to send the current method to the instrument

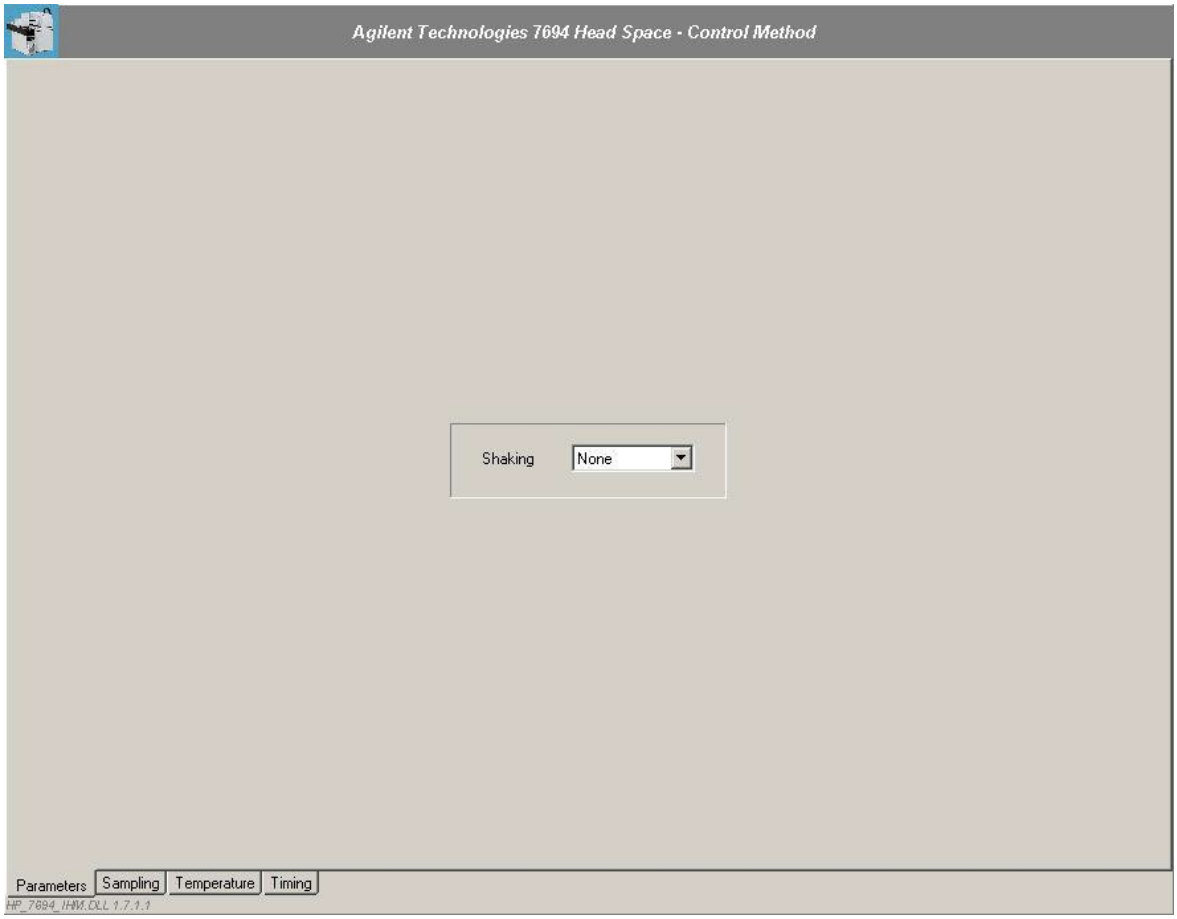
to get the active method from the instrument

to print the current method

Click on the button to display the Agilent 7694 Headspace Autosampler control method section.

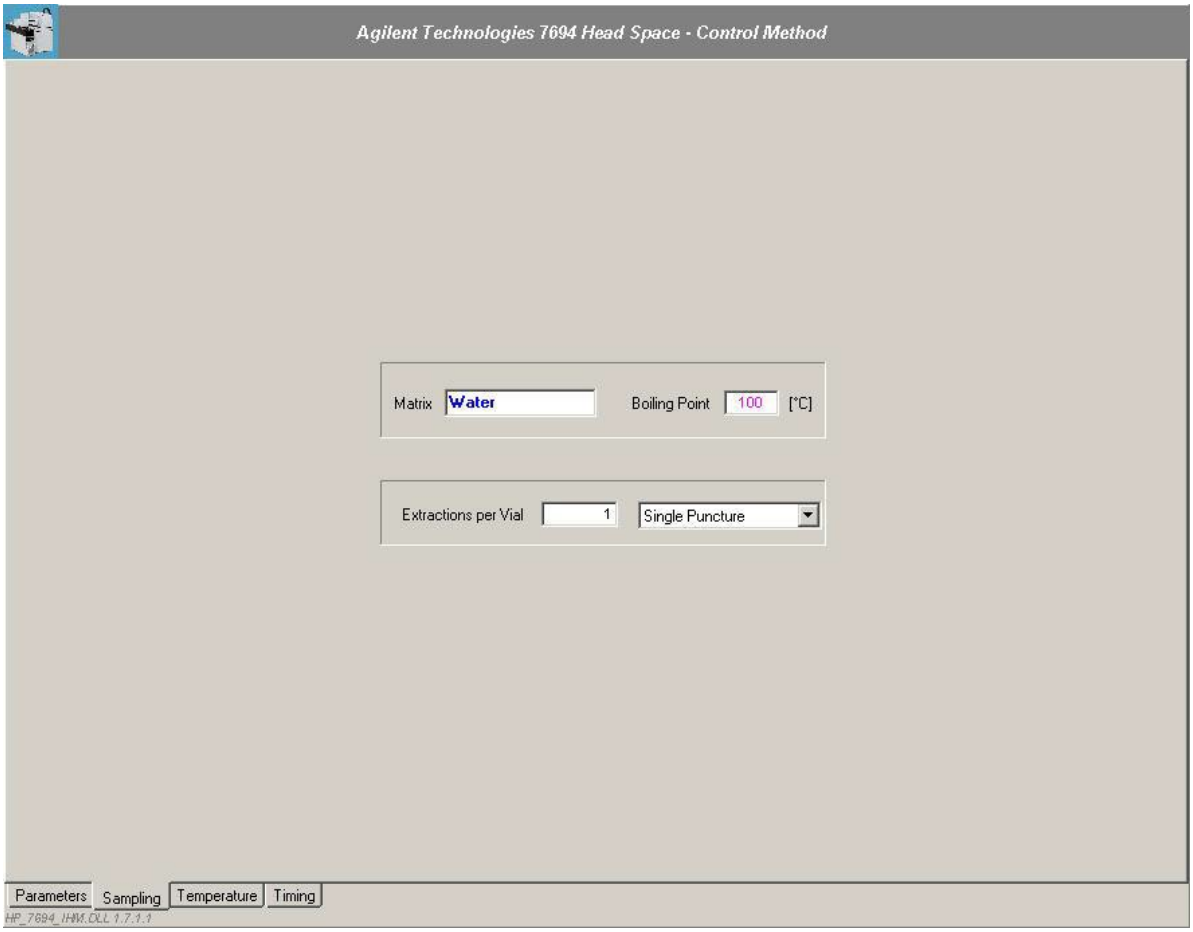
It contains four sub-sections: Parameters, Sampling, Temperature and Timing. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Parameters Control



Shaking: Select the agitation level of oven carousel during vial equilibration: None, Low or High.

Sampling Control



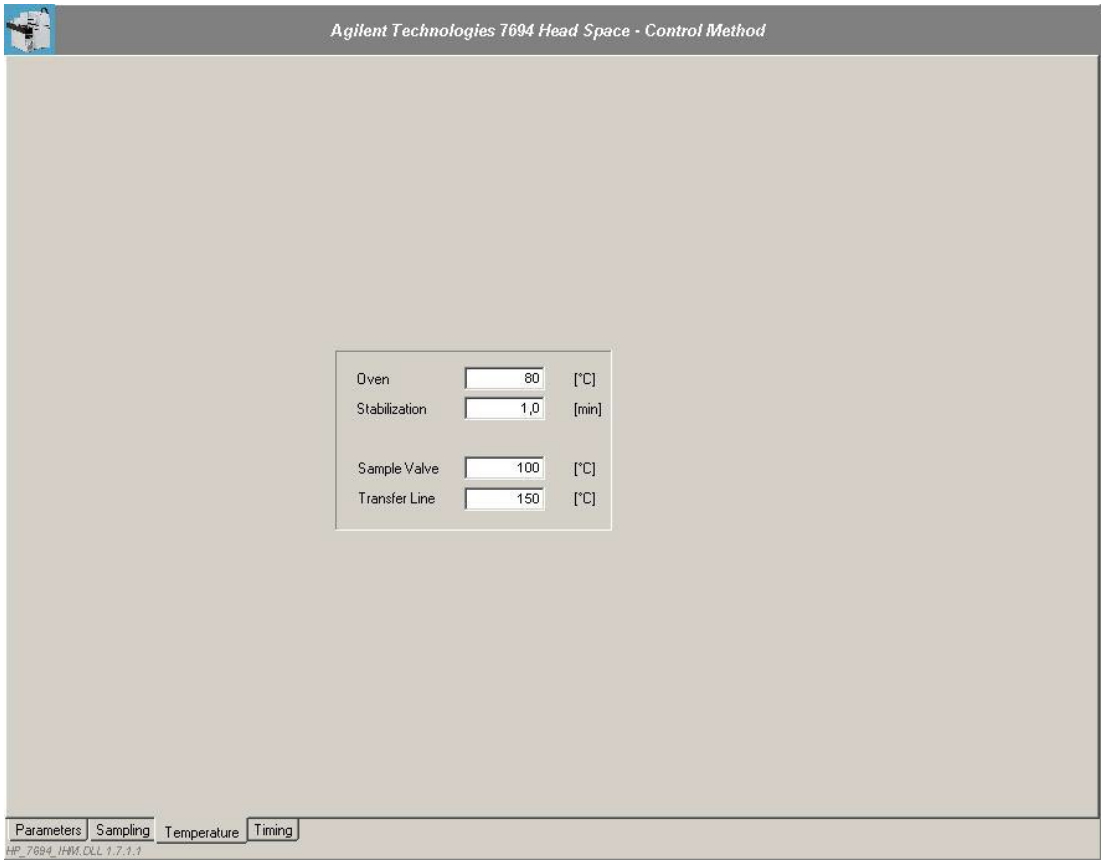
Matrix: Enter in this field the matrix of the sample.

Boiling point: Enter in this field the boiling point of the sample.

The two previous fields are only information fields not used by the instrument

Extractions per Vial: Enter in this field the number of extraction to do per sample. When the number exceeds one, select in the dropdown list the puncture mode. Two choices are available single puncture and multiple puncture.

Temperature Control



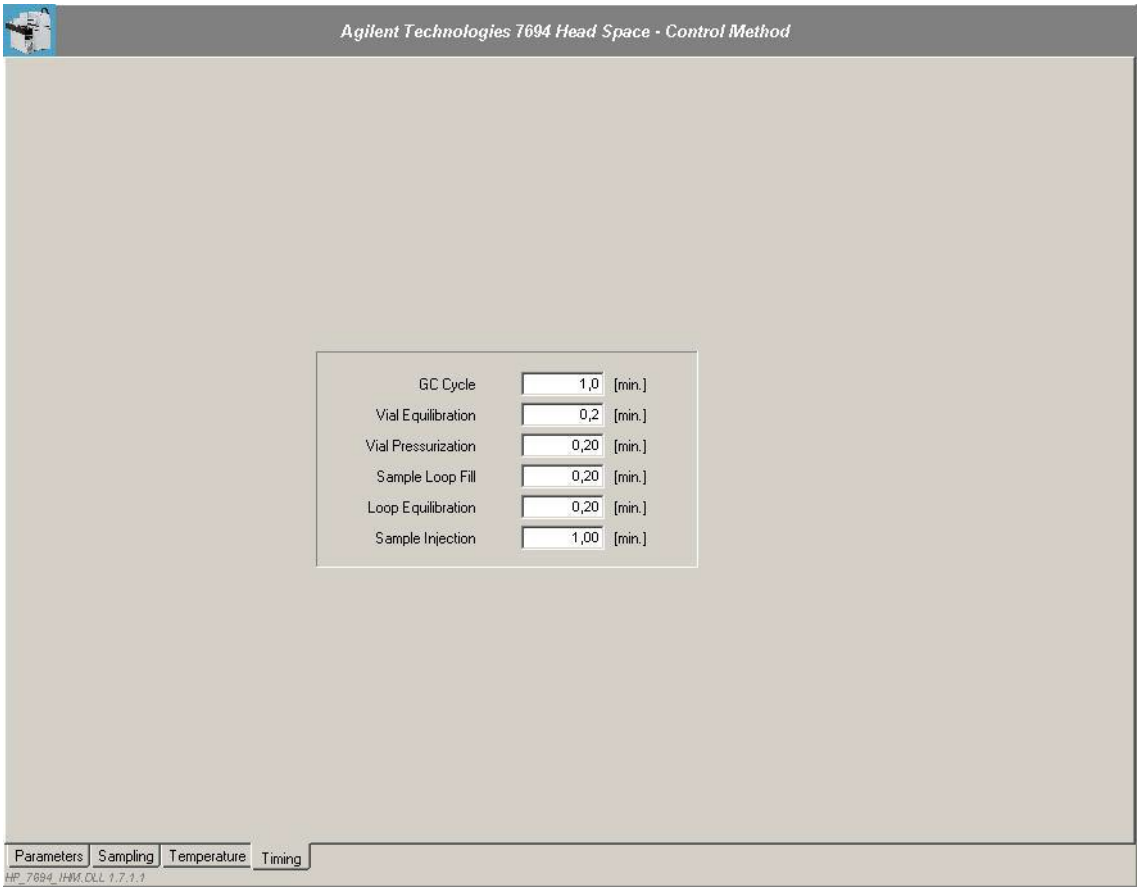
Oven: Enter in this field the temperature of the oven where the vials are prepared.

Stabilization: Enter in this field the temperature stabilization time of the oven.

Sample Valve: Enter in this field the sample loop temperature.

Transfer Line: Enter in this field the transfer line temperature.

Timing Control



GC Cycle: Enter in this field the time for the total GC run to complete. (Total run includes the GC run and cool–down time and the vial equilibration time.)

Vial Equilibration: Enter in this field the vial equilibration time which is the time the sample vial spends heating in the oven to form the headspace gas.

Vial Pressurization: Enter in this field the pressurization time. It specifies the time that gas is allowed to enter the vial through the sampling needle to build up additional pressure in the vial.

Sample Loop Fill: Enter in this field the sample loop fill time. It is the time during which the vent valve is open. The gases in the sample vial travel through the sample loop and are vented to the outside. This fills the sample loop with a precise aliquot of headspace gas.

Loop Equilibration: Enter in this field the loop equilibration time. It is the time after the vent valve closes during which the gases in the sample loop equilibrate with the pressure and temperature of the sample loop.

Sample Injection: Enter in this field the sample injection time. It is the time in which the sample valve is open and the gases in the sample loop are swept into the GC.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

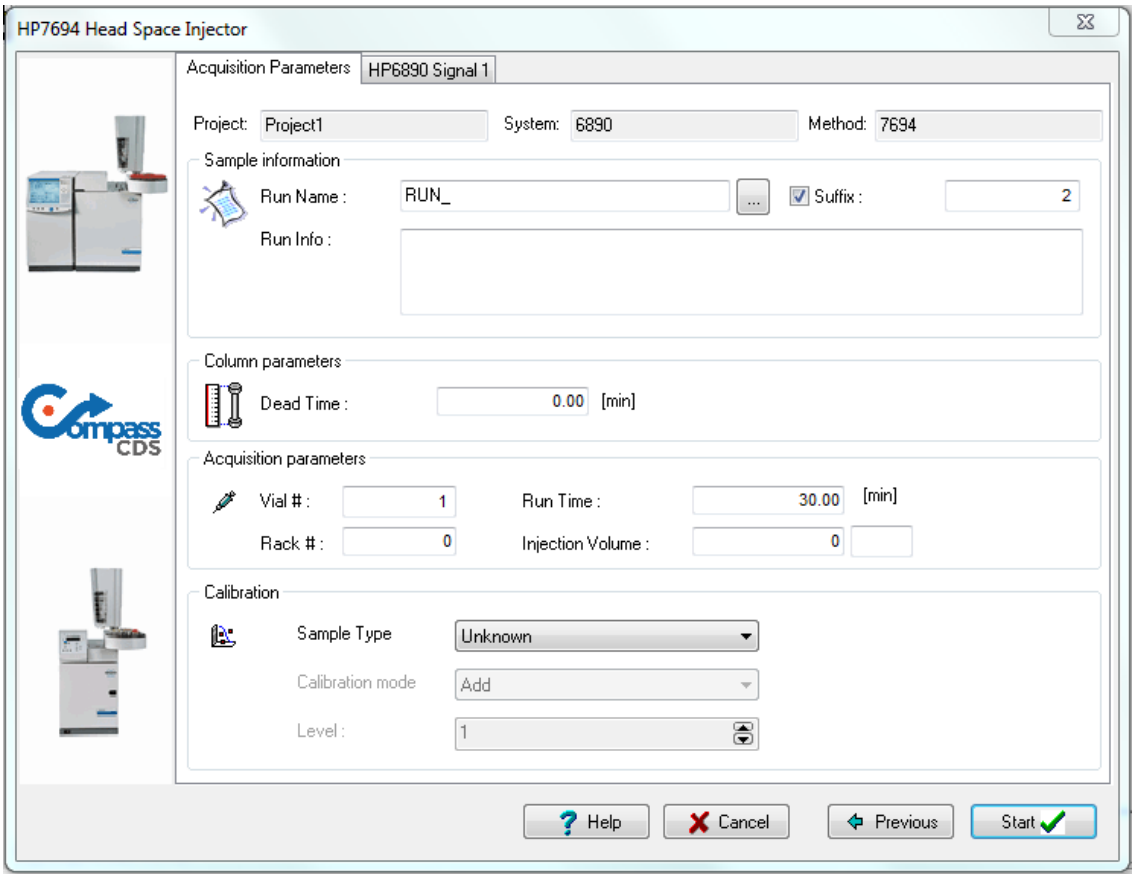
Quick Start (Single Acquisition)

Press the button.

In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

Press the OK button.

The following screen is displayed:



In the *Acquisition parameters* tab, required fields like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

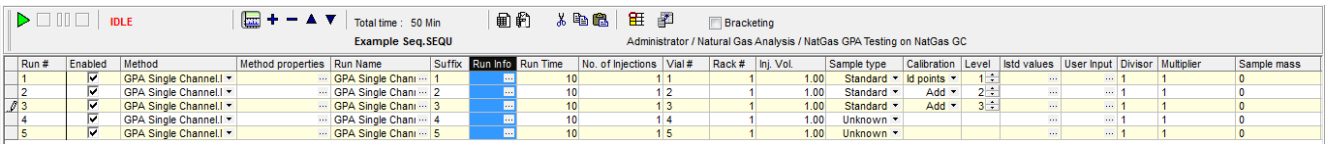
Other parameters associated with each acquisition channel can be entered in the Channel X tab.

Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data System User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS User Guide).



Run #	Enabled	Method	Method properties	Run Name	Suffix	Run Info	Run Time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type	Calibration	Level	Istd values	User Input	Divisor	Multiplier	Sample mass
1	☑	GPA Single Channel.I	...	GPA Single Chani	1	...	10	1	1	1	1.00	Standard	Id points	1	...	...	1	1	0
2	☑	GPA Single Channel.I	...	GPA Single Chani	2	...	10	1	2	1	1.00	Standard	Add	2	...	...	1	1	0
3	☑	GPA Single Channel.I	...	GPA Single Chani	3	...	10	1	3	1	1.00	Standard	Add	3	...	...	1	1	0
4	☑	GPA Single Channel.I	...	GPA Single Chani	4	...	10	1	4	1	1.00	Unknown			...	...	1	1	0
5	☑	GPA Single Channel.I	...	GPA Single Chani	5	...	10	1	5	1	1.00	Unknown			...	...	1	1	0

The *Method Name*, the *Run Name*, the *Run ID,* and the *Acquisition length* must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS User Guide.

Running Acquisition Status

Viewing a Running Acquisition

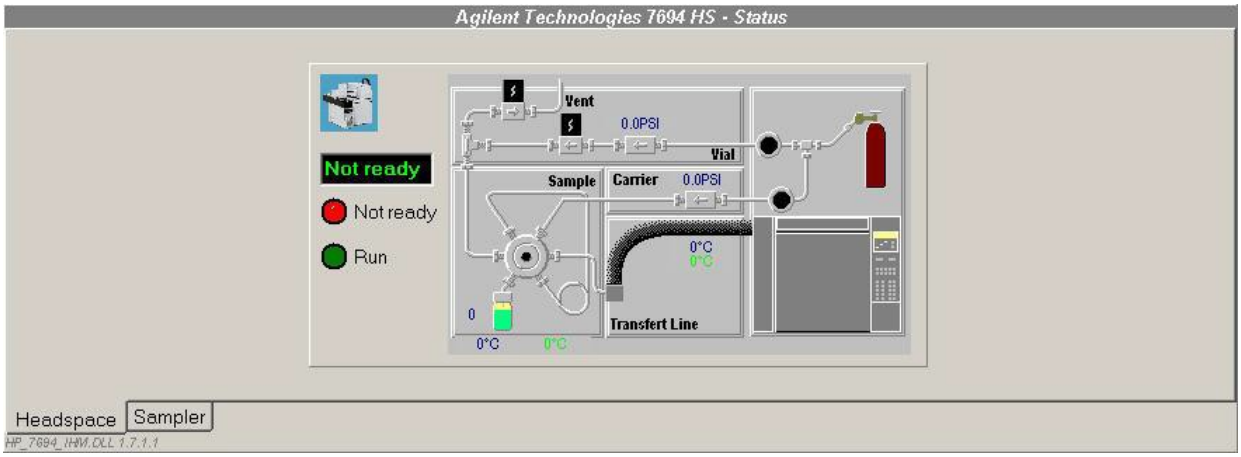
To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Agilent 7694 Headspace Autosampler

Click on the

button corresponding to the Agilent 7694 Headspace Autosampler driver and the Agilent Technologies 7694 Headspace Autosampler status screen will appear. It contains two sub-sections: *Headspace and Sampler.* Click on the required sub-section to display the corresponding screen.

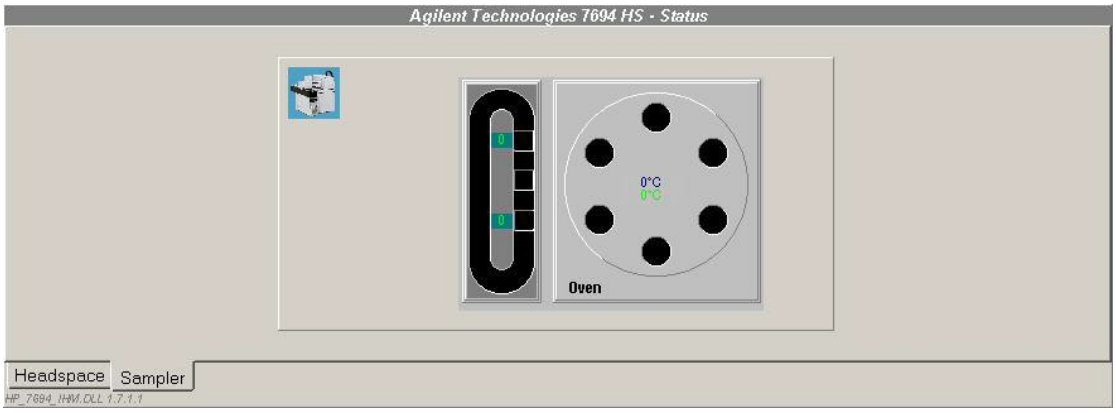
Headspace Status



This is a read-only window.

Information like temperatures and pressures of the instrument are displayed.

Sampler Status



This is a read-only window.

This screen displays the status of the vial in the oven.

Overview Window

Click on the Over View button: for this driver, nothing is displayed.

Agilent 6890 & 6850 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501552
Revision C

Contents

Introduction 3
Installation and Configuration 3
  Installing the Driver Software 3
  Configuring the GC Communications 3
    Serial Communications 3
    Ethernet Communications 3
  Configuring the Driver 4
    Configuring the Agilent 6890 Gas Chromatograph 4
Building a Method 11
  Creating a New Method 11
  Control Method Section for the Agilent 6890 Gas Chromatograph 13
    Sampler Control 14
    Oven Control 15
    Cryo Control 16
    Aux Control 16
    Valves Control 18
    Events Control 20
    Column Control 21
    Inlet Control 23
    Cool On Column 25
    HP – Programmable Temperature Vaporization 27
    Gerstel Programmable Temperature Vaporization 29
    Pressure Control Module (PCM) 30
  Detector Control 31
    FID (Flame Ionization Detector) 31
    TCD (Thermal Conductivity Detector) 32
    NPD (Nitrogen-Phosphorus Detector) 33
    ECD (Electron Capture Detector) 34
    µECD (micro Electron Capture Detector) 35
Starting and Viewing an Acquisition 36
  Quick Start and Sequence 36
    Quick Start (Single Acquisition) 36
    Sequence 37
  Running Acquisition Status 37
    Viewing a Running Acquisition 37
    Status of the Agilent 6890 Gas Chromatograph 38
Appendix 43
  Injection Volumes 43
  Configuring a Fixed IP address 46

Introduction

This document describes the configuration of the Agilent Technologies 6890 GC driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and what actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Driver software, refer to the CompassCDS installation Guide.

Configuring the GC Communications

Serial Communications

The Agilent Technologies 6890 Gas Chromatograph uses RS232 protocol as the method of communications for instrument control and for sending digital data to the external data system.

The serial connection is made at the back at the 6890 GC.

Serial communication is standard on all Agilent 6890 or 6850 GCs.

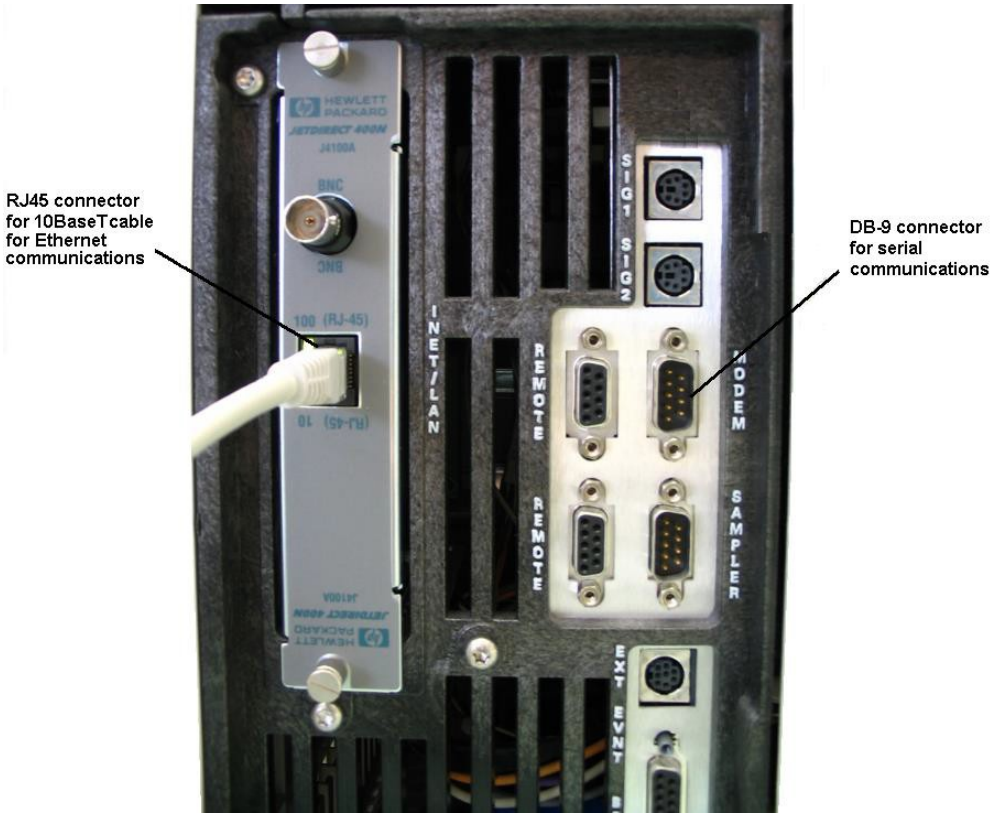
Ethernet Communications

The Agilent 6890 Gas Chromatograph uses Ethernet® as the method of communications for instrument control and for sending digital data to the external data system.

Ethernet communication is standard on the Agilent 6890 GC.

The Ethernet connection is made at the back at the 6890 GC. There are two types of Ethernet cables

- An Ethernet crossover cable is used when the Agilent 6890 GC is connected directly to the CompassCDS Acquisition Server PC.
- A standard Ethernet patch cable is used when the Agilent 6890 GC is connected to a company Ethernet network.



The Agilent 6890 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server or a DHCP server is used to send IP addresses to TCP/IP devices.

The BOOTP Server lists Ethernet addresses along with the IP addresses that are to be assigned to the corresponding devices.

To know how to configure the BOOTP server, refer to the CompassCDS installation Guide.

It is also possible to give a fixed IP address to the GC. To know how to fix the IP address of the GC, refer to the 6890 GC manual.

NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

Configuring the Driver

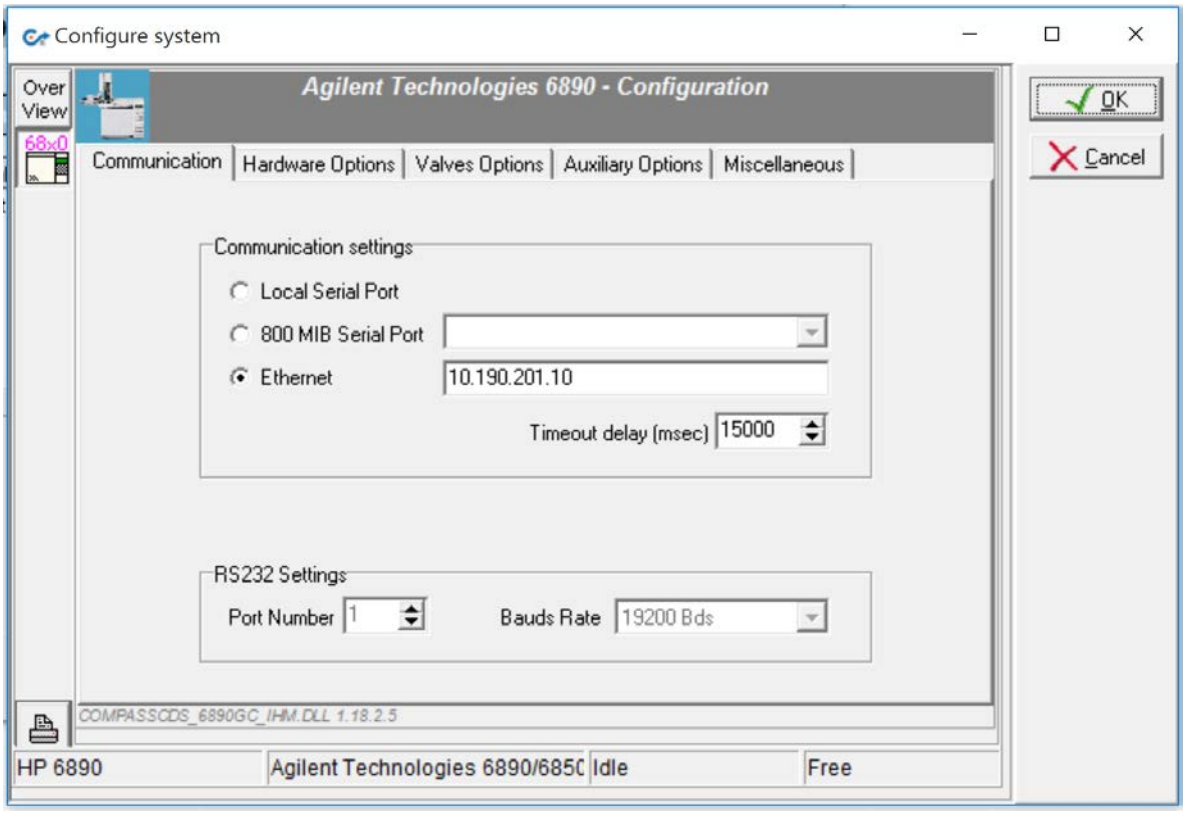
The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Agilent 6890 Gas Chromatograph

Click on the

button corresponding to the Agilent 6890 GC driver and the configuration screen appears.

Communication Window



Communication settings Parameter Group

Local Serial Port

Select this option if the chromatograph is connected directly to the serial port of the PC.

STAR 800 & 850 MIB Serial Port:

Select this option and then the name of the STAR 800 & 850 MIB interface used to connect to the chromatograph.

Ethernet

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

NOTE: If you will be using the Serial port installed in the STAR 800 & 850 MIB interface, configure the MIB-interface module before configuring the Agilent Technologies 6890 Gas Chromatograph driver.

RS232 settings Parameter Group

Port Number

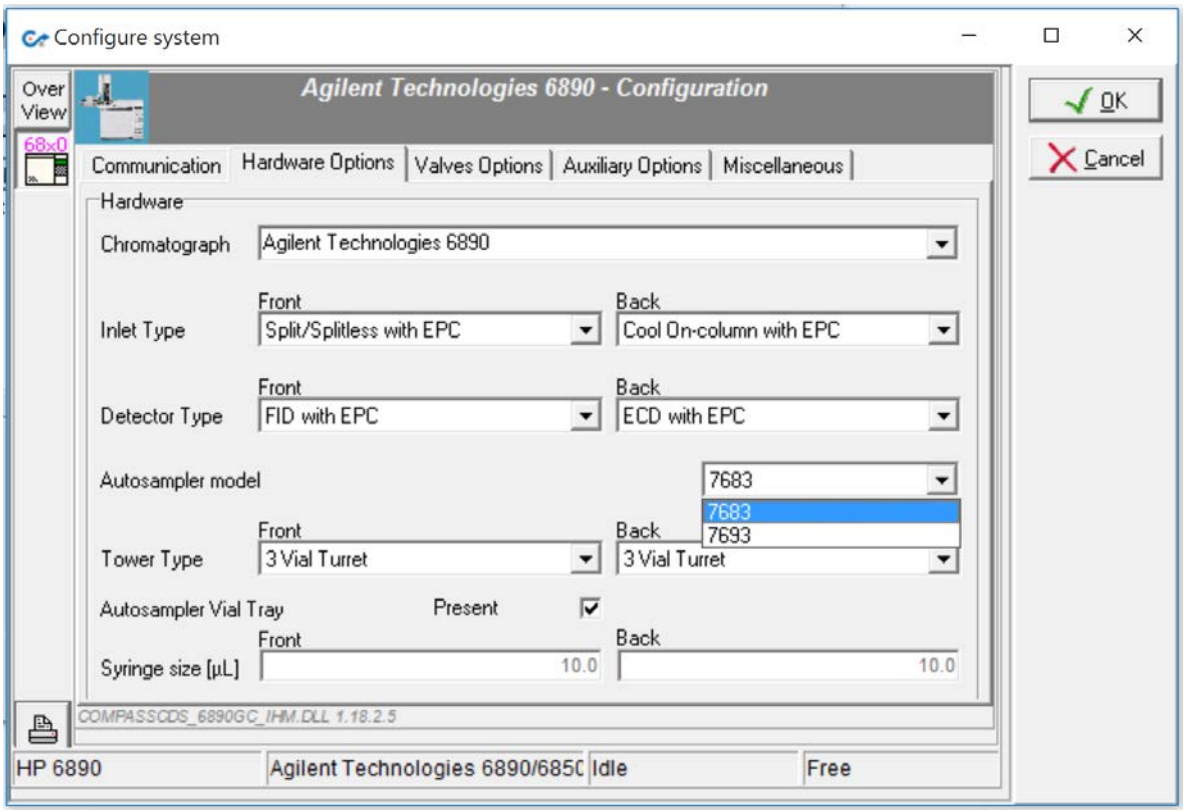
Select the PC or STAR 800 & 850 interface Serial port number on which the chromatograph will be connected.

Baud Rate

Select the baud rate to communicate with the GC. Two choices are available 19200 or 9600.

To determine the baud rate of the GC, refer to the appendix Configuring the GC RS232 communication.

Hardware Options Window



Hardware Parameter Group

Chromatograph

Select the *Chromatograph* model. Available choices are: Agilent Technologies 6890, Agilent Technologies 6890 Plus, Agilent Technologies 6850.

The back inlet, detector and sampler options are available only for Agilent Technologies 6890 and Agilent Technologies 6890 Plus. Only one inlet, one detector and one sampler can be configured with an Agilent 6850 GC.

Front and Back Inlet Type

Select the *Front* and *Back Inlet Type*. The available choices are: None, Purged packed, Purged packed with EPC, Cool On-Column, Cool On-Column with EPC, Split/Splitless, Split/Splitless with EPC, Gerstel CIS3 PTV with EPC, Gerstel CIS4 PTV with EPC, PTV with EPC, PCM, PCM with heater.

Front and Back Detector type

Select the *Front* and *Back Detector Type*. The available choices are: None, FID, FID with EPC, TCD, TCD with EPC, NPD and NPD with EPC.

Autosampler Type

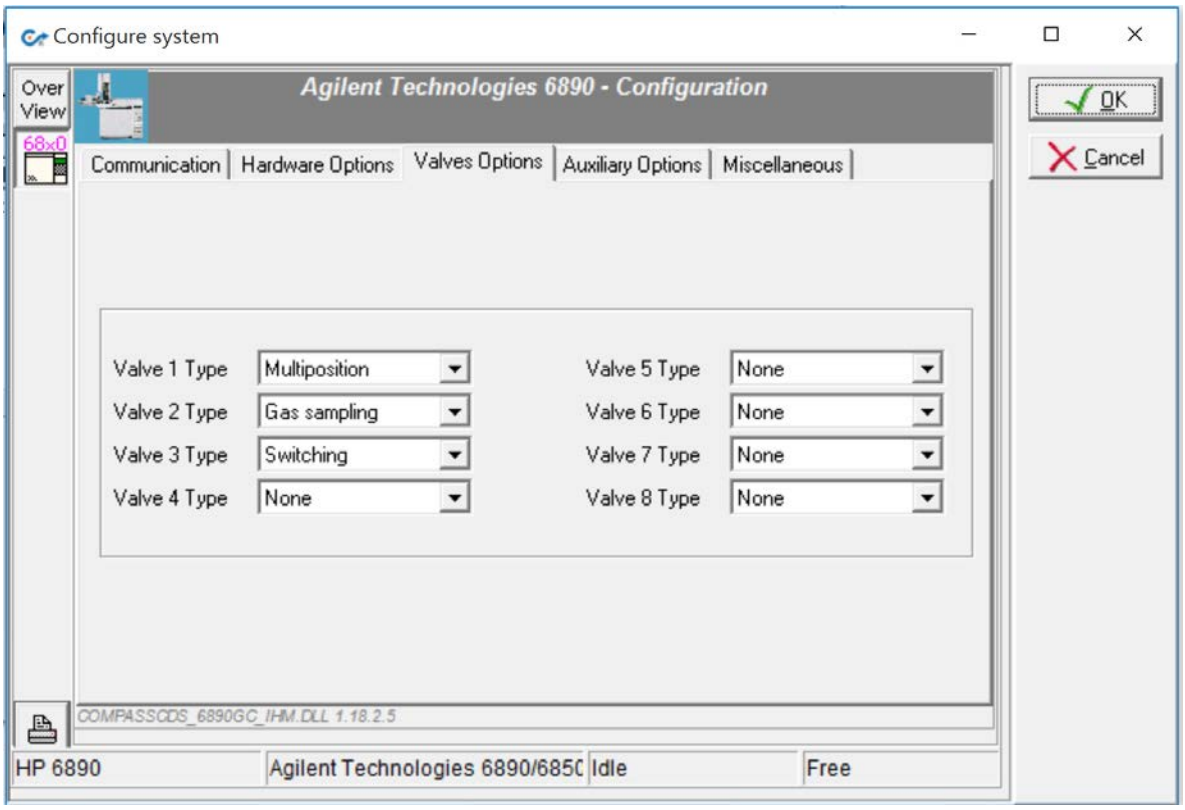
Select either Autosampler 7683 (old model) or 7693 (new model). For the 7693 autosampler a syringe volume has to be entered for the front and back Autosampler position.

Front and Back Sampler Type

Select the *Front* and *Back Sampler Type*. The available choices are: None, 3 Vial Turret, 8 Vial Turret, 22 (2 mL) Vial Turret, 27 (4 mL) Vial Turret.

Check *Present* if the chromatographic system is equipped with a 100 Vial Tray.

Valves Options Window

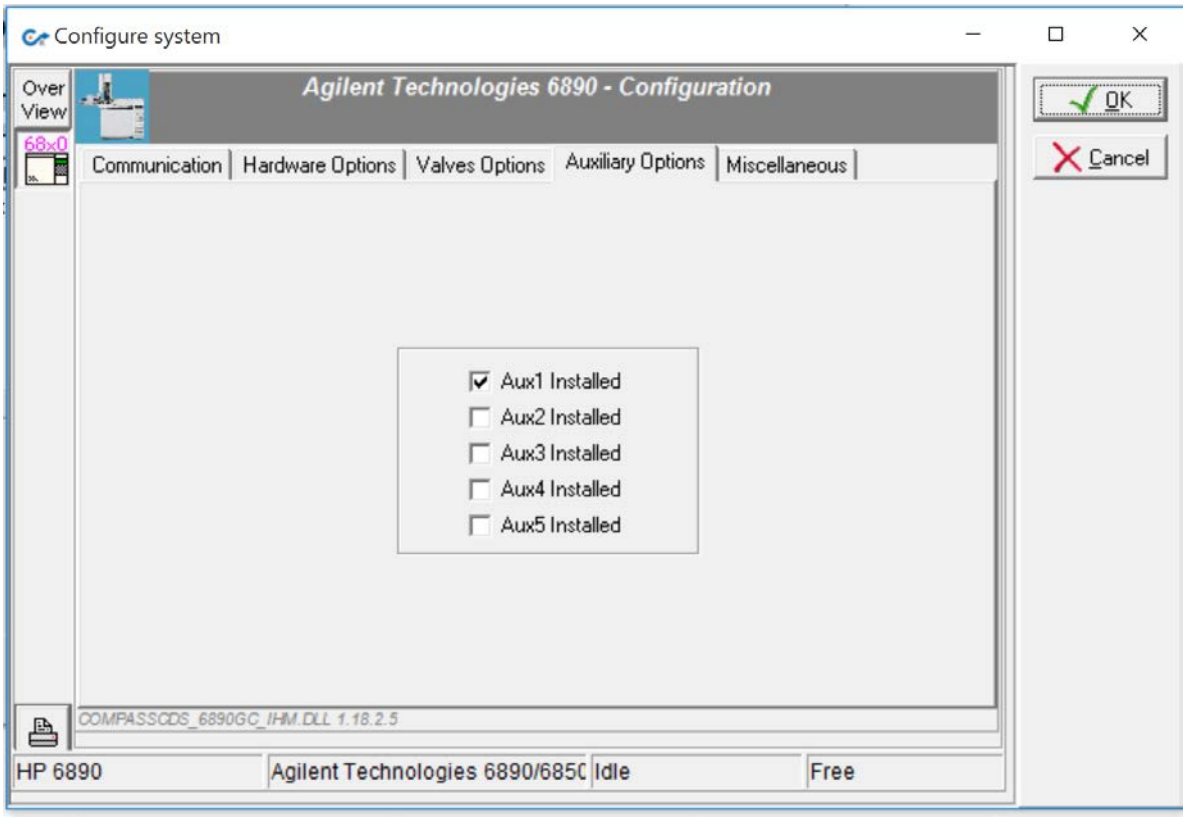


The user can configure up to 8 valves.

Select the *Valve Type*. Four choices are available: *None*, *Multiposition*, *Gas sampling*, *Switching*.

- Multiposition: Generally used as a gas stream selection valve, to select one of several gas streams.
- Gas sampling: A run is automatically started when the valve switches from load position to inject position.
- Switching: Generally used to select one of two columns for analysis.

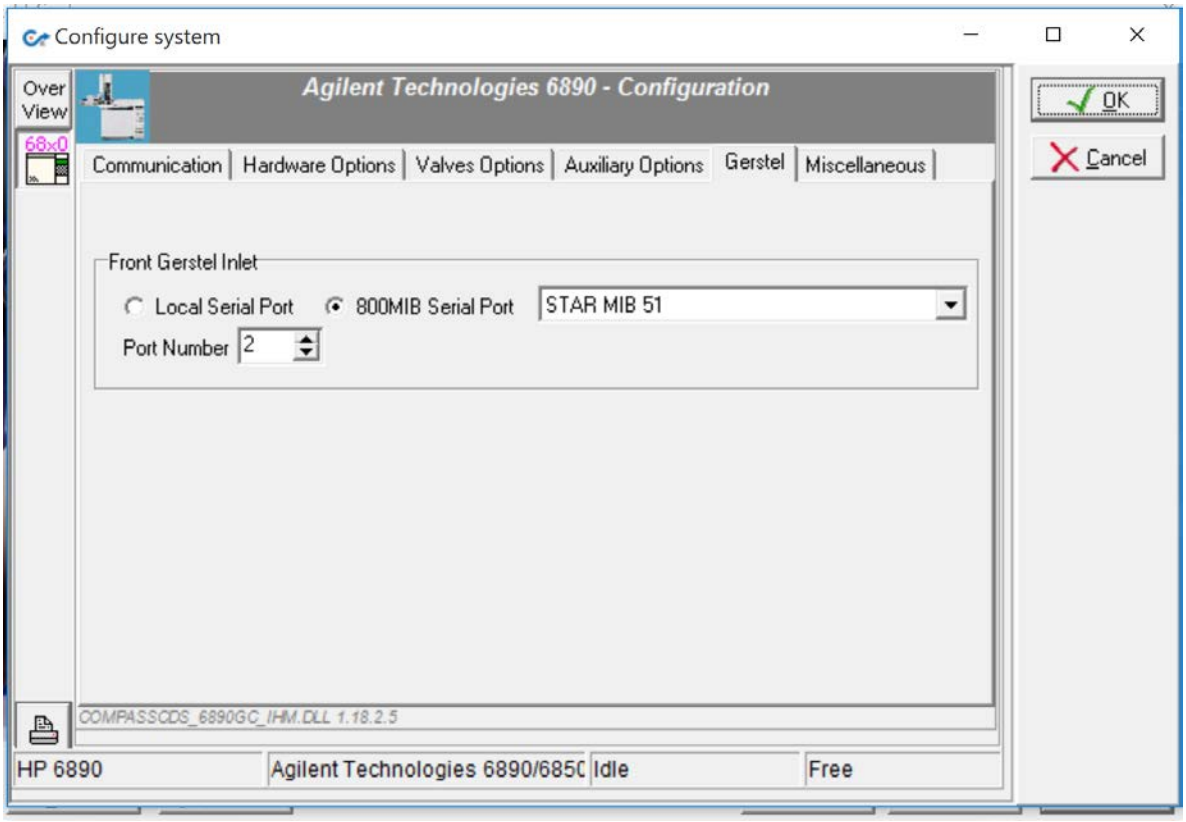
Auxiliary Options Window



This instrument gives the user the choice of two extra heating blocks (Aux 1 and 2) (for example, to heat a retention- gap) and three additional pneumatics (Aux 3, 4 and 5). Check the corresponding box(es)

To save the configuration, click on the *OK* button. Then right click on the system name in the bottom part of the *CompassCDS Configuration Manager* browser. A pop-up menu appears: click on *Stop.* Then right click on the system name again, and click on *Start.*

Gerstel Window



Front/Back Gerstel Inlet Parameter Group

Local Serial Port

Select this option if the Gerstel controller is connected directly to the PC.

STAR 800 & 850 MIB Serial Port:

Select this option and then the name of the MIB-interface used to connect to the Gerstel controller.

Port Number: COM

Select the PC or STAR 800 & 850 interface Serial port number on which the Gerstel controller will be connected.

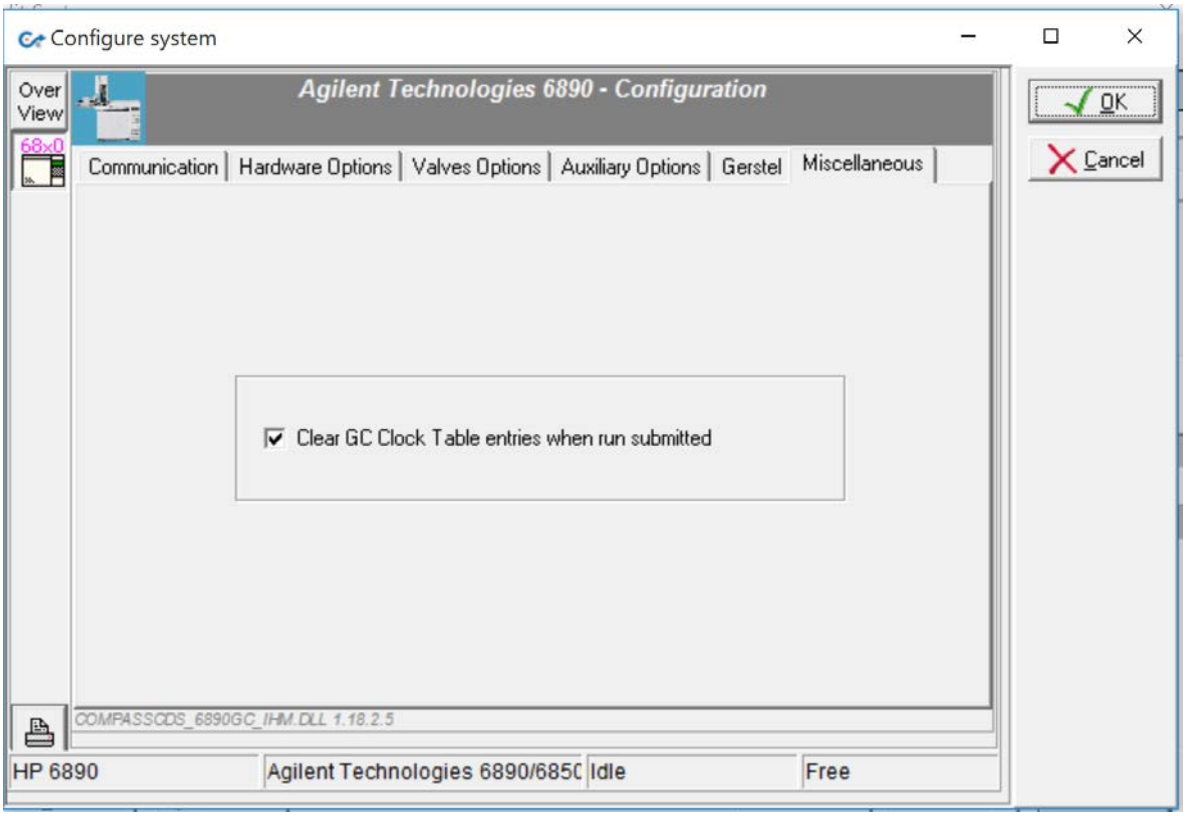
NOTE: If you will be using the Serial port installed in the STAR 800 & 850 interface, configure the MIB-interface module before configuring the Agilent Technologies 6890 Gas Chromatograph driver.

For more information about the configuration of the MIB-interface, refer to the STAR 800 & 850 Interface MIB User Guide.

NOTE: Once the system has been created and correctly configured, it must be associated to one or several projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration.

Miscellaneous Window



Clear GC Clock Table entries when run submitted

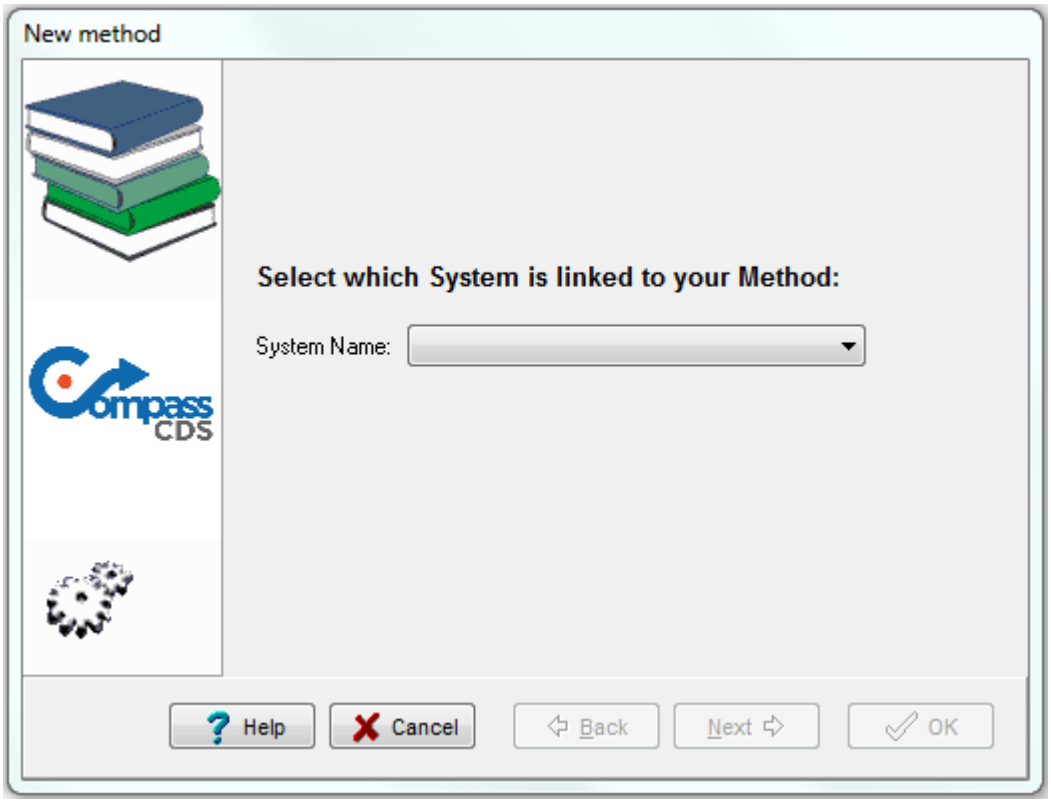
Check this option if you want to clear the GC Clock Table prior to each run. The GC Clock Table give the ability to activate a GC method at a certain time, start a run at a certain time of the day… As such event can interact with CompassCDS activity, it is recommended to clear the GC Clock Table priority to each run.

Building a Method

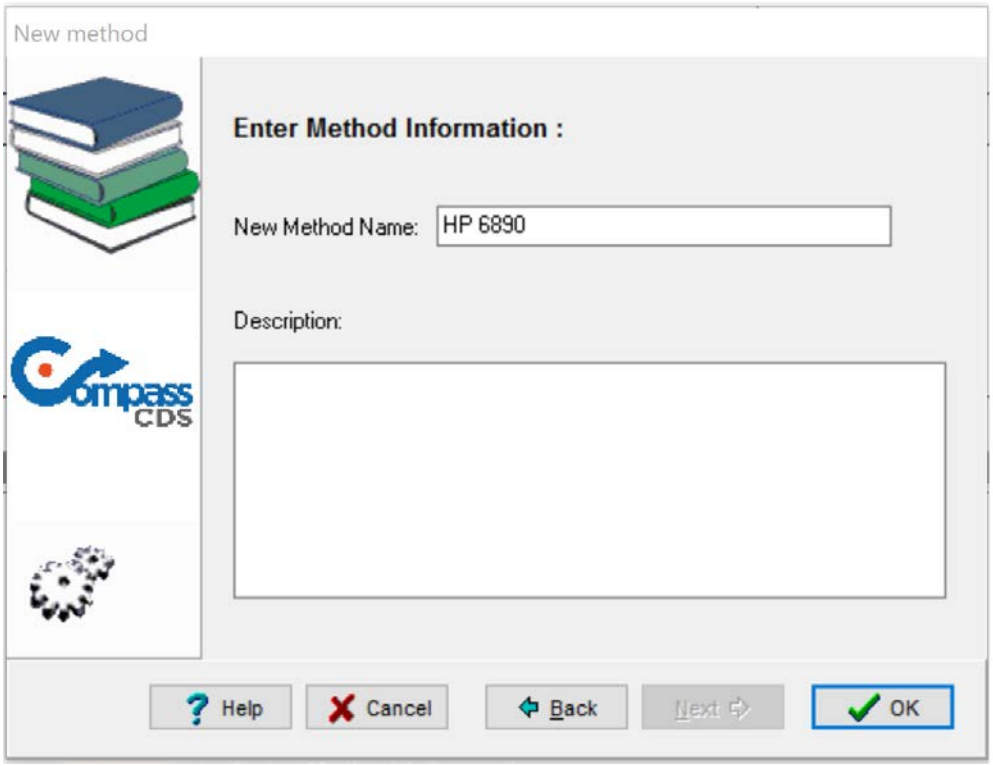
Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

1. To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS Chromatography Data System main menu.
   A wizard guide will appear and provide assistance during the first steps of method creation



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.
3. Once this field is completed, click on the Next button to move to the second step of the method creation



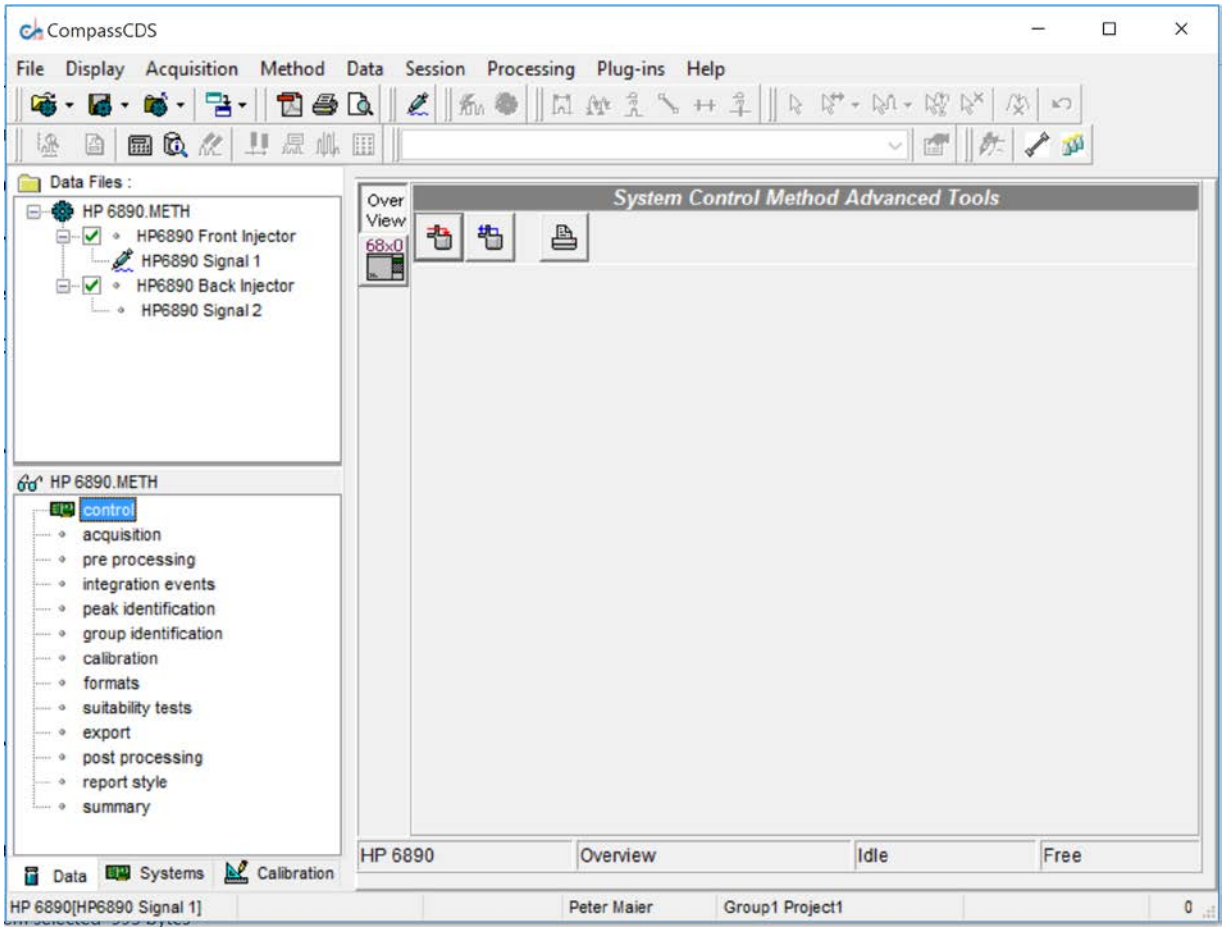
4. Enter the *New Method Name* in the first field. In the *Description* field, enter information concerning the method (optional).
5. Once these two fields have been completed, click on the *OK* button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

The control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Agilent 6890 Gas Chromatograph is detailed. Other parameters such as *Injection Volume*, *Vial* and *Rack* number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to the CompassCDS Chromatography Data System User Guide.

Control Method Section for the Agilent 6890 Gas Chromatograph

Once the new method is created, select the control section in the lower part of the browser. The following screen appears



Press the Over View button to display the ***System Control Method Advanced Tools*** window

to send the current method to the instrument

to get the active method from the instrument

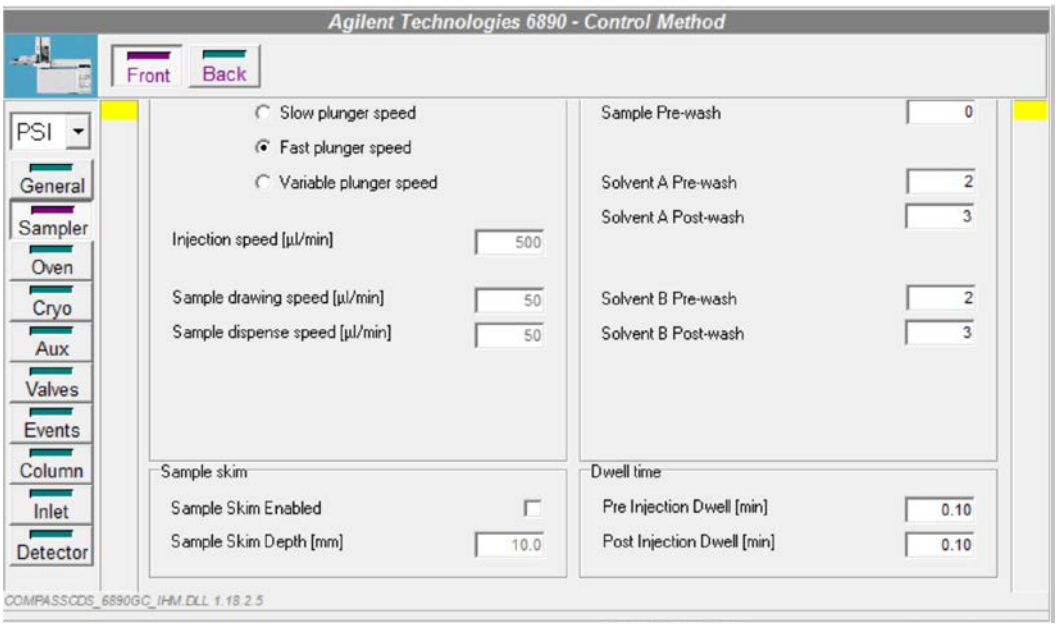
to print the current method

Click on the button to display the Agilent 6890 Gas Chromatograph control method section.

It contains 8 sub-sections: *General, sampler, Oven, Cryo, Events, Column, Inlet and Detector*. Up to two additional sub-sections can be also activated depending on the system configuration: *Aux* (if *Auxiliaries* have been configured), and *Valves* (if *Valves* have been configured). Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

A scrolling list in the left top corner allows you to choose the pressure unit. The available choices are: *bar*, *psi*, *kPa*. A *Send* button sends the program parameters to the GC.

Sampler Control



Depending on the system configuration, select the *Front* or *Back* button, to set the sampler information of each sub-system.

NOTE: The Agilent Technologies 6850 Gas Chromatograph has only one sub-system. Therefore, only the *Front* information should be set.

Select the *Active* box to activate and take into account the *Sampler parameters*.

In the *Sample Pumps* field, enter the number of pumps before the injection (plunger strokes to avoid the formation of bubbles). The allowed range is 0–15.

In the *Viscosity Delay* field, enter a time (in seconds). During this time, the syringe plunger has a pause between the pumping and the injection stroke. For viscous samples, the pause allows the sample to flow into the vacuum created in the syringe. The allowed range is 0–7.

In the *Sample Pre-wash* field, enter the number of syringe washes with the sample, before injection. The allowed range is 0-15.

In the *Solvent A* and *B Pre-wash*, enter the number of syringe washes with solvent A and/or B, before injection. The allowed range is 0–15.

In the *Pre Injection Dwell Time,* enter the time the needle stays in the inlet before the injection. In the *Post Injection Dwell Time*, enter the time the needle stays in the inlet after the injection. Check *Sample Skim Enabled* if you want to modify the position of the needle in the sample vial.

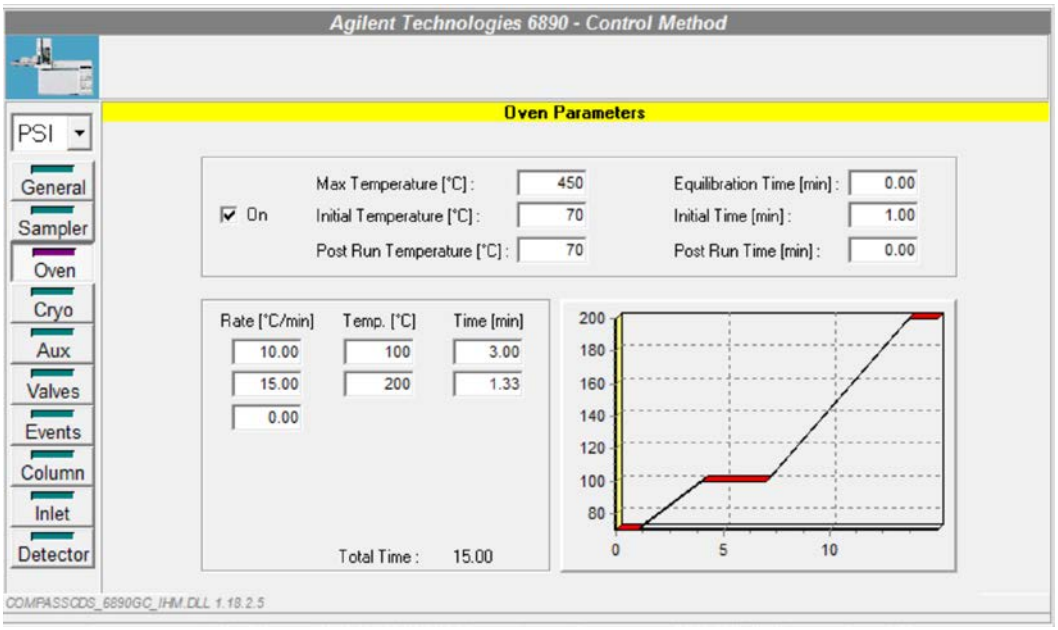
In the *Sample Skim Depth,* enter the difference between the default needle position in the sample vial and the desired one (negative or positive values).

In the *Solvent A* and *B Post-wash*, enter the number of syringe washes with solvent A and/or B, after injection. The allowed range is 0–15.

Select the plunger speed during the injection. Three choices are available: *Slow Plunger Speed, Fast Plunger Speed* or *Variable Plunger Speed*. If *Variable Plunger Speed* is selected, three additional values should be entered, the *Drawing Speed*, the *Dispense speed* and the *Injection Speed*.

NOTE: The volume that will be injected depends of the syringe size. Only five levels of injection volume for the 6890 and six levels for the 6850 can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4, 5 and (6). These values represent the number of tenth of the syringe volume. For example, if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 10^{nth}= 3 µL. A physical turret option called *Nanoliter* allows the injection of smaller volume (refer to the Agilent manual to know more about this option). Refer to the Appendix (*Injection Volumes* section) to see the correspondence between the programmed levels and the real injected volumes.

Oven Control



Check the *On* box to activate the oven programming.

In the *Max Temperature* field, enter the column maximum temperature in °C.

In the *Equilibration Time* field, enter the time before the GC becomes ready in minutes. In the *Initial Temperature* field, enter the column initial temperature in °C.

In the *Initial Time* field, enter the time the GC stays at the *Initial Temperature* (first plateau) in minutes.

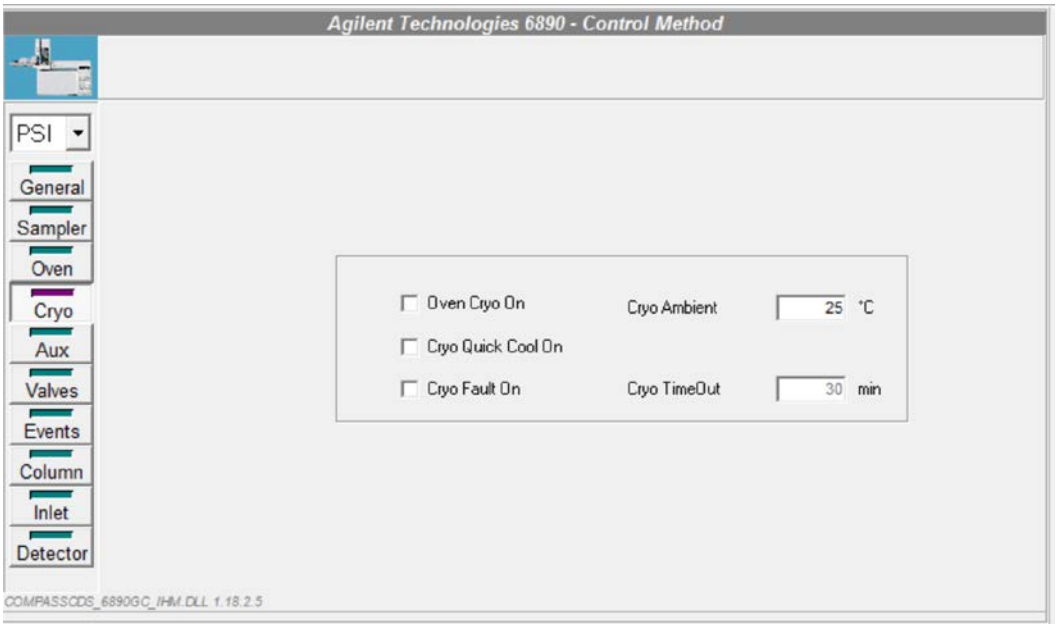
In the *Post Run Temperature* field, enter the temperature which is maintained in the column after the analysis.

In the *Post Run Time* field, enter the time the GC maintains the *Post Run Temperature* in the column after the analysis in the table program the rates, the plateau temperatures, and the duration of the oven plateau temperature.

The graphic to the right side of the table displays the oven temperature program.

The total time of the oven program is displayed in the *Total Time* field.

Cryo Control



The cryogenic system generates an oven temperature lower than the ambient temperature.

Check the *Oven Cryo On* box to activate the cryogenic system for the column oven. Enter the ambient temperature in the *Cryo Ambient* field. Below this temperature, column oven cryogenics will be used.

Check *Cryo Quick Cool On* to quickly cool the oven after a run.

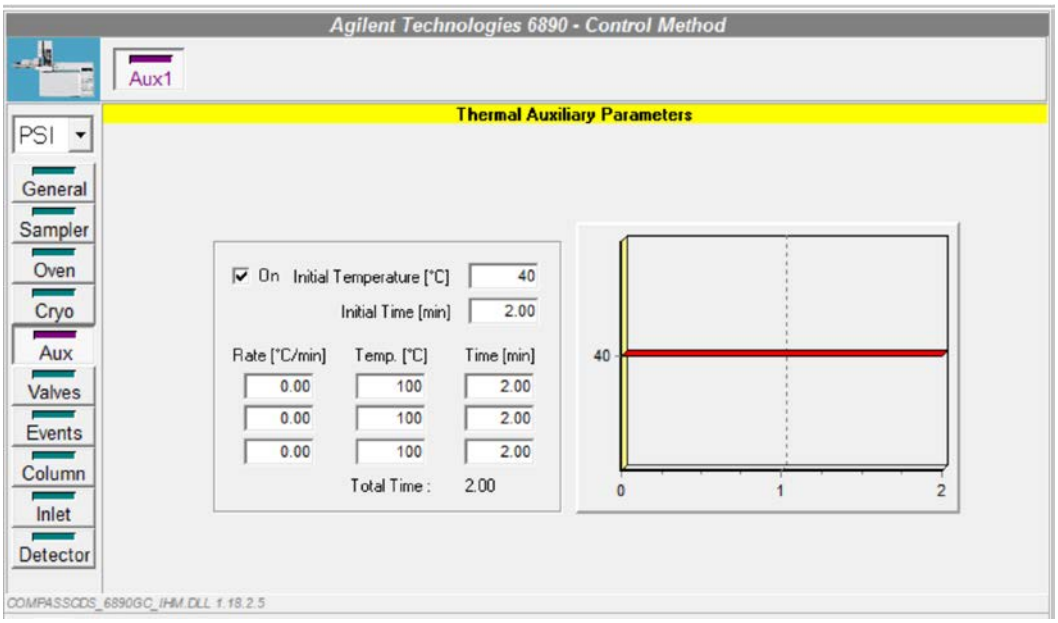
Check *Cryo Fault On* to stop the oven after 17 minutes if the cryogenic system has not reached the desired temperature. The oven stops if no injection is started before the time entered in the *Cryo Timeout* field.

Aux Control

The instrument allows to configure two heater blocks (Aux 1 and 2) and three pressure control channels (Aux 3, 4 and 5).

This sub-section is active only when at least one auxiliary is configured for the system in the CompassCDS Configuration Manager. The different fields depend on system configuration.

Thermal Auxiliary Parameters



Check the *On* box to enable temperature programming.

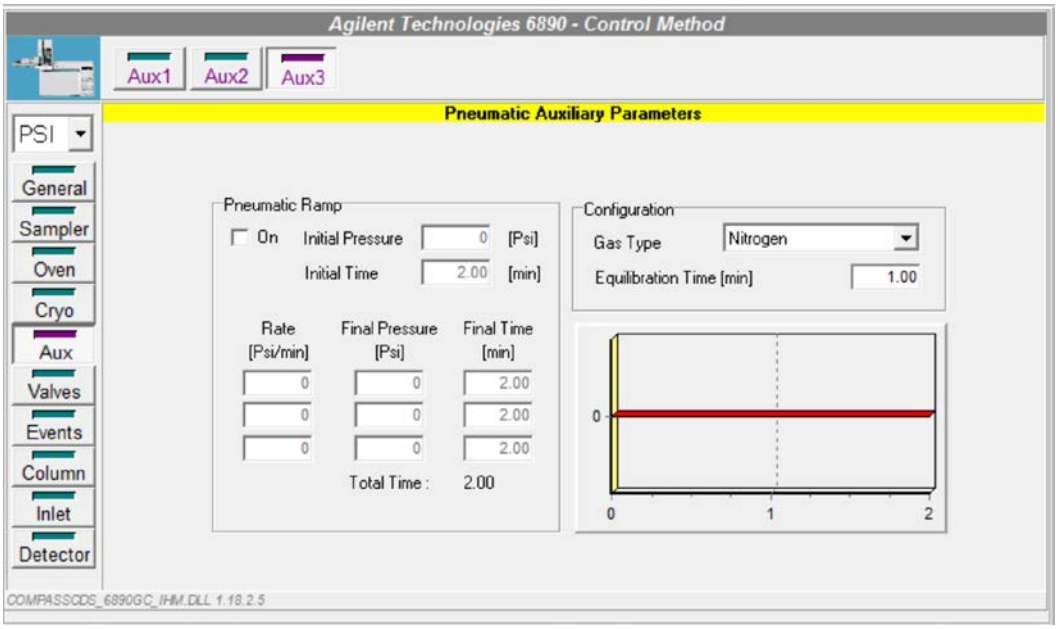
In the *Initial Temperature* field, enter the initial temperature in °C.

In the *Initial Time* field, enter the time the heater block stays to the *Initial Temperature* (first plateau) in minutes.

In the table program the rates, the plateau temperatures, and the duration of the heater block plateau temperature. The graphic to the right of the table displays the temperature program.

The total time of the heater block program is displayed in the *Total Time* field.

Pneumatic Auxiliary Parameters



Pneumatic Ramp Parameter Group

Check the On box to enable pressure programming. In the Initial Pressure field, enter the initial pressure.

The pressure units will be those shown in the list box in the top left corner of the 6890 method window.

In the Initial Time field, enter the time for this first plateau in minutes.

In the table in minutes, program the rates, the plateau pressure, and the duration of the plateau pressure. The figure on the right side displays the pressure program.

The total time of the program is displayed in the Total Time field.

Configuration Parameter Group

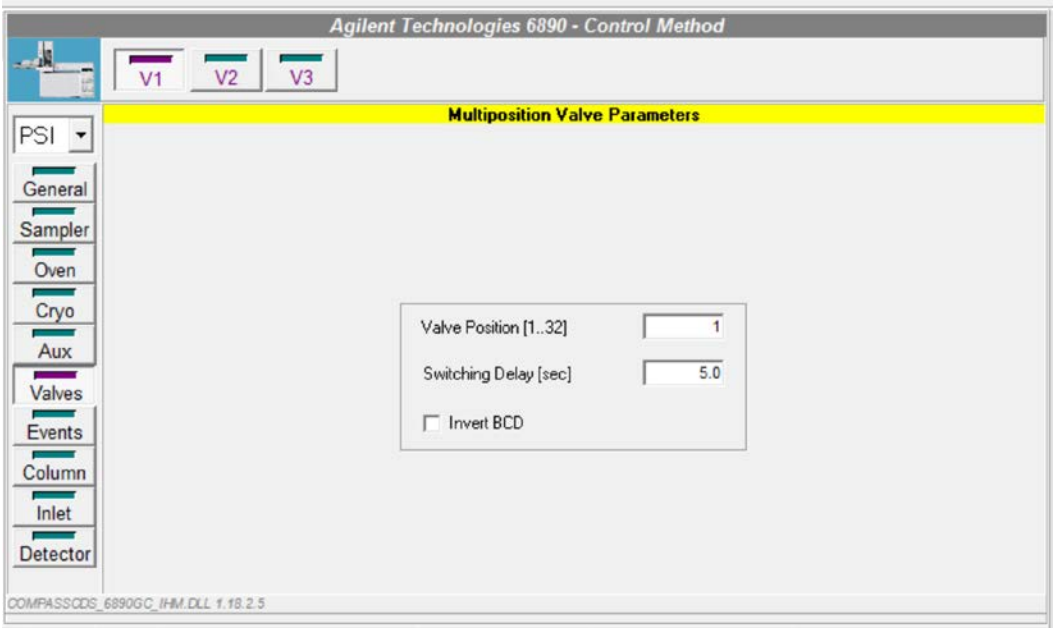
Select the Gas type. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, Unknown.

In the Equilibration Time field, enter the time before the auxiliary becomes ready.

Valves Control

The instrument can have up to eight valves configured. The different fields depend on system configuration. Three types of valves exist: *gas samling, multiposition*, and *switching valves*.

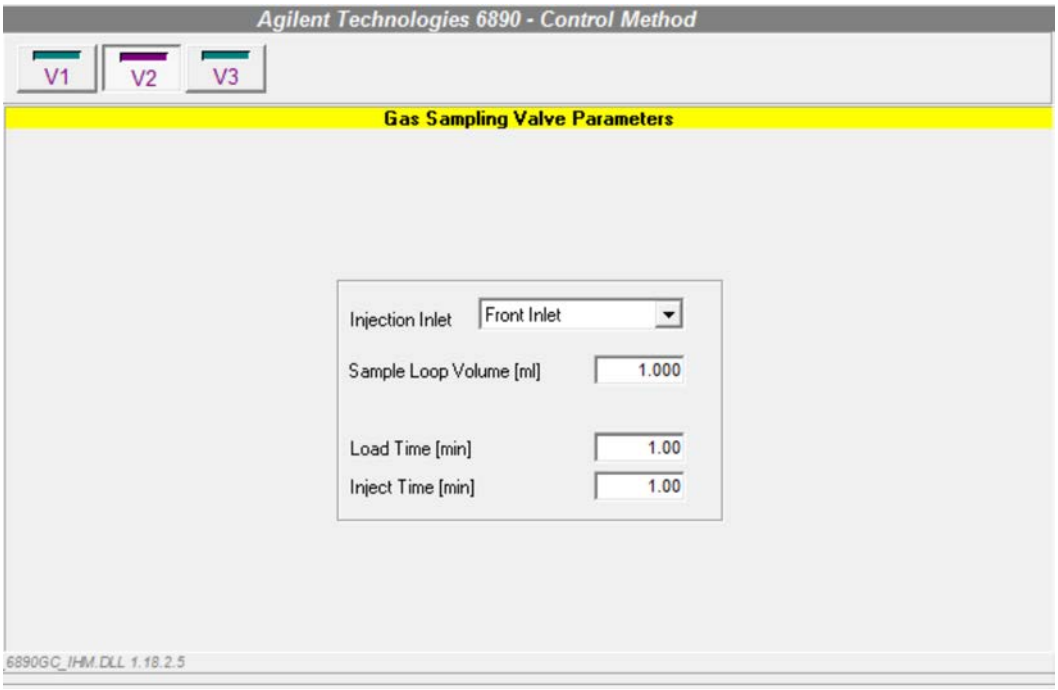
Multiposition Valve Parameters



In the Valve Position field, enter the initial position of the valve among 32 positions. In the Switching Delay field, enter the time between the valve switches.

Check the Invert BCD checkbox to invert the valves codes.

Gas Sampling Valve Parameters



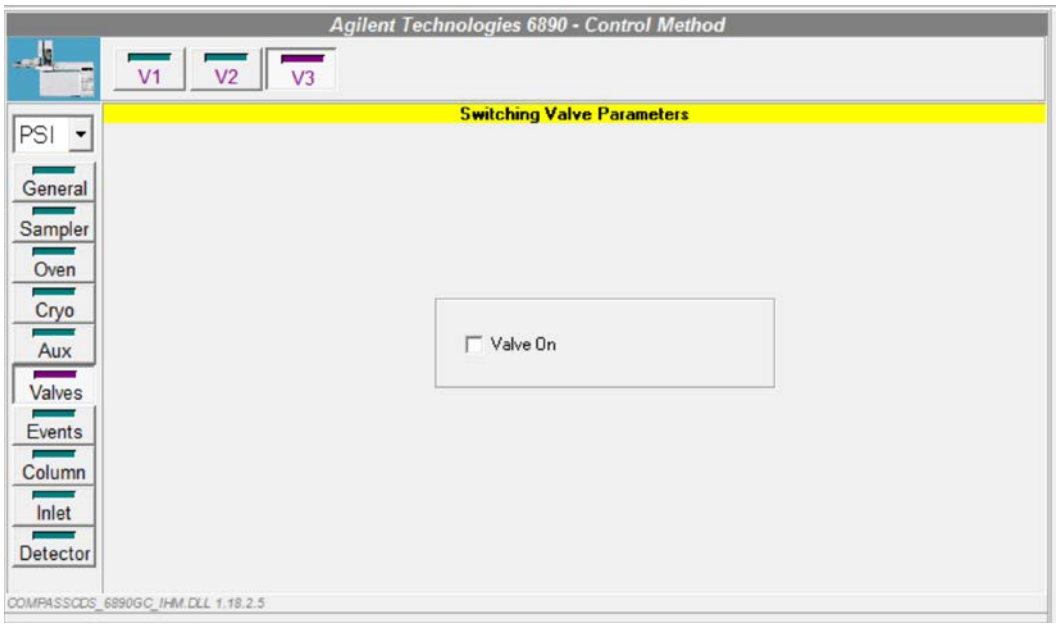
Select the *Injection Inlet* which is connected to the gas sampling valve. The available choices are: *Front Inlet*, *Back Inlet*, *Aux3*, *Aux4*, *Aux5*.

In the *Sample loop volume* field, enter the loop volume in mL.

In the *Load time* field, enter the time the valve stays in load position.

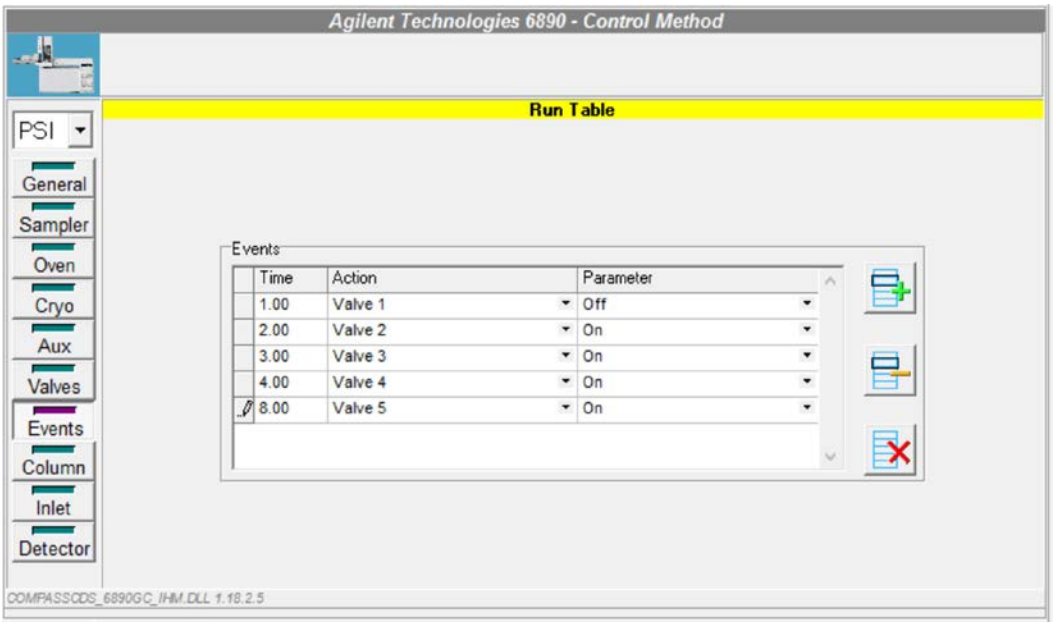
In the *Inject time* field, enter the time the valve stays in inject position. As soon as the inject time begins, the acquisition starts.

Switching Valve Parameters



Check the Valve On checkbox to activate the valve. It allows the switching of the valve from one position to another. An event must be added in the event table to switch the valve.

Events Control



In this table program events like valve switching, signal range, and attenuation, autozero, TCD

polarity change, etc.

NOTE: If the valve rotation is programmed with the event table, it would be better to program the initial position at the end of the analysis.

Use the following buttons to edit the table

to add a line to the table

to delete a line in the table

to clear the entire table

In the Time column enter the time when the action has to be done.

In the Action column, select the action to do. The available choices are

Valve 1	Signal 1 zero	Signal 2 Resume
Valve 2	Signal 1 attenuation	Aux 3 pressure
Valve 3	Signal 1 range	Aux 4 pressure
Valve 4	Signal 1 Freeze	Aux 5 pressure
Valve 5	Signal 1 Resume	Front TCD Invert Polarity
Valve 6	Signal 2 zero	Back TCD Invert Polarity
Valve 7	Signal 2 attenuation	Front NPD Fuel
Valve 8	Signal 2 range	Gas Back NPD Fuel Gas
Multi-position valve	Signal 2 Freeze	

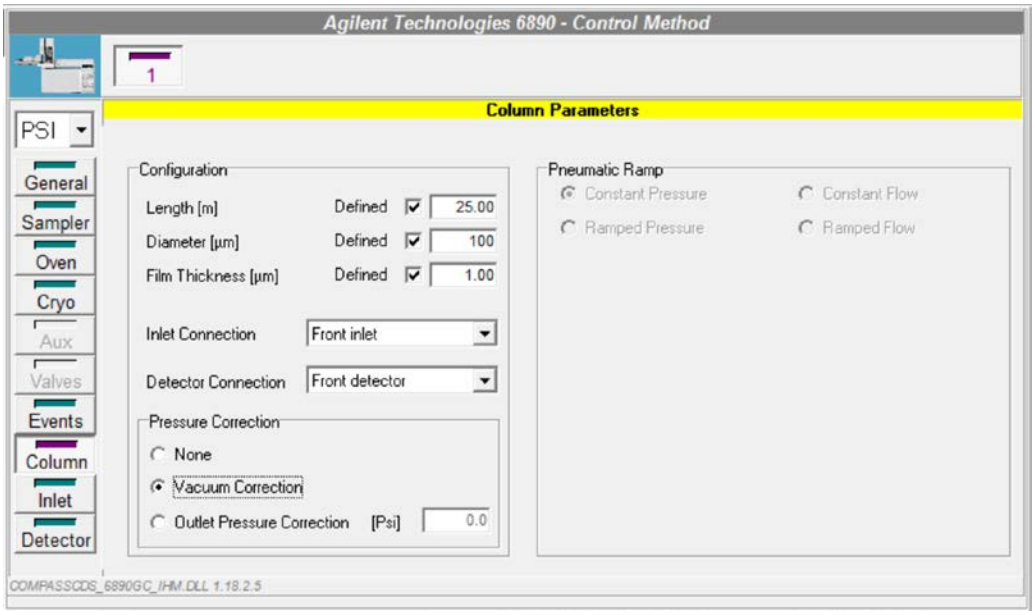
In the *Parameter* column, select if the valve is switched *On* or *Off* at the specified time.

Column Control

Depending on the system configuration, select the *1 or 2* button, to set the column information of each sub-system.

NOTE: The Agilent Technologies 6850 Gas Chromatograph has only one sub-system. Therefore, only the *1* information must be set.

The different fields depend on system configuration.



Configuration Parameter Group

In the Length field, enter the column length in meters, if Defined box is checked.

In the Diameter field, enter the column diameter in microns, if Defined box is checked.

In the Film Thickness field, enter the column film thickness in microns, if Defined box is checked.

Select the Inlet Connection. The available choices are: Front inlet, Back inlet, aux3, Aux4, Aux 5, Unknown.

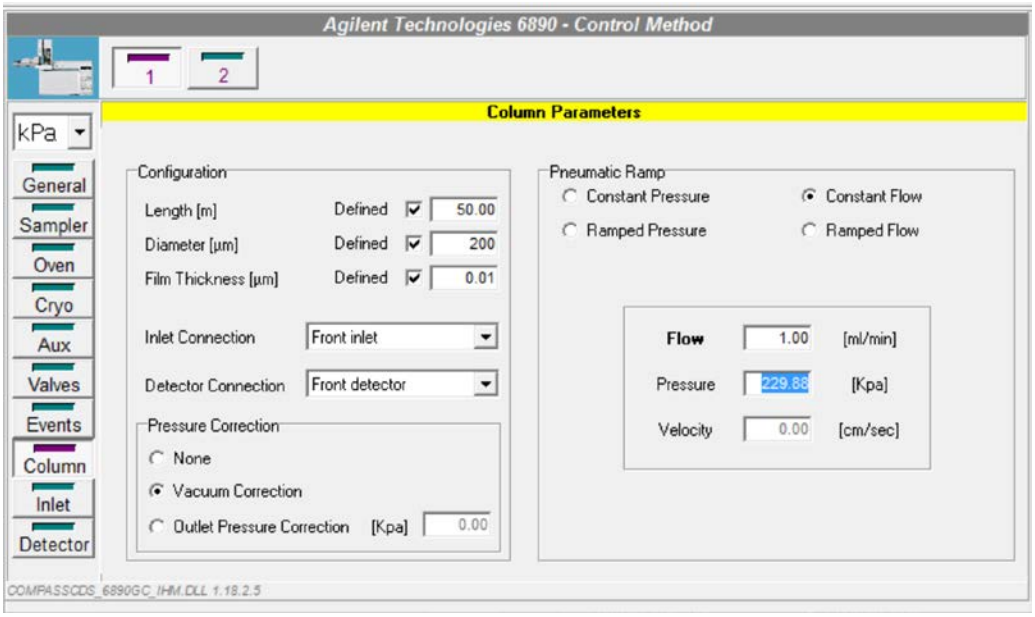
Select the Detector Connection. The available choices are: Front detector, Back detector, MSD (Mass Spectrometry Detector), AED (Atomic Emission Detector), Others.

Check the Vacuum Correction box to correct the output pressure, when the column is connected to a detector which pressure is lower than the atmospheric one (MSD).

Check the Outlet Pressure Correction box to correct the output pressure, when the column is connected to an AED. Enter the pressure of the detector.

Pneumatic Ramp Parameter Group

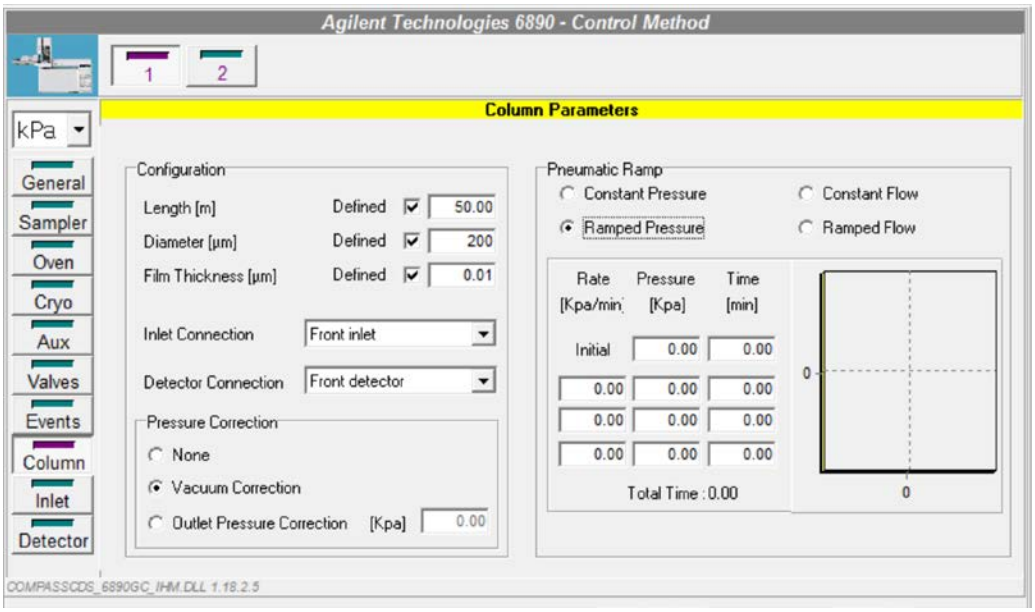
These parameters are active only if the inlet is controlled by an EPC (Aux3, Aux4, Aux5 or Inlet with EPC).



Check the Constant Pressure to maintain a constant pressure in the column. Then enter the corresponding pressure or flow in the Pressure or Flow fields.

Check the Constant Flow to maintain a constant flow in the column. Then enter the corresponding flow or pressure in the Flow or Pressure fields.

The velocity is displayed in the Velocity field.



Check the Ramped Pressure to set a pressure program.

In the table program the rate, the plateau pressure, and the duration of the column plateau pressure. The graphic to the right of the table displays the pressure program.

The total time of the program is displayed in the Total Time field. Check the Ramped Flow to set a flow program in the column.

In the table program the rate, the plateau flow, and the duration of the column plateau flow. The graphic to the right of the table program displays flow program.

The total time of the program is displayed in the Total Time field.

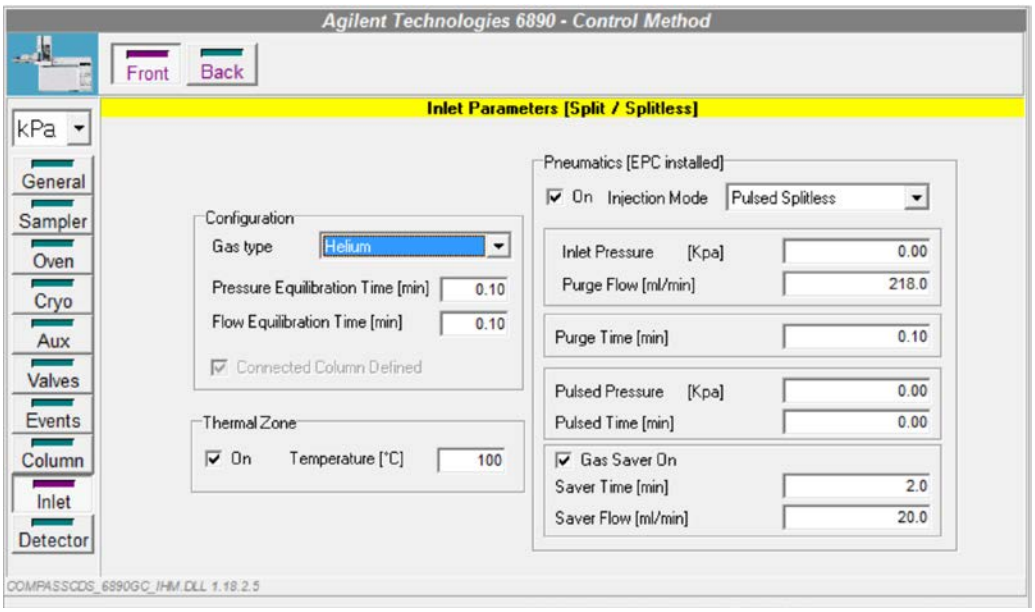
Inlet Control

Depending on the system configuration, select the Front or Back button, to set the inlet information of each sub-system.

NOTE: The Agilent Technologies 6850 Gas Chromatograph has only one sub-system. Therefore, only the Front information should be set.

The different fields depend on system configuration.

Split/Splitless



Configuration Parameter Group

Select the Gas type. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, and Unknown.

In the Pressure Equilibration Time, enter the time before the inlet pressure becomes ready. In the Flow Equilibration Time, enter the time before the inlet flow becomes ready.

The Connected Column Defined field is selected if the column configuration has been defined in the Column Parameters sub-section.

Thermal Zone Parameter Group

Check the On box to activate the inlet temperature. Enter the desired Temperature.

Pneumatic Parameter Group

Check the On box to activate the pneumatic parameters.

Select the Injection mode. The available choices are: Split, Splitless, Pulsed split and Pulsed splitless. According to this choice, the following parameters are activated or not.

In the Inlet Pressure field, enter the pressure of the inlet.

In the Split Ratio field, enter the ratio between the flow division and column flow. This field is available only if the

Split and *Pulsed Split* inlets are selected.

In the Purge flow field, enter the flow of the purge vent in mL/min. This field is available only if the Splitless and

Pulsed Splitless inlets are selected.

In the Total Flow field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined in the Column Parameters sub-section.

In the Purge Time field, enter the time the purge valve is opened. This field is available only if the Splitless and Pulsed Splitless inlets are selected.

In the Pulsed Pressure field, enter the inlet pressure when the acquisition starts. This field is available only if the Pulsed Split and Pulsed Splitless inlets are selected.

In the Pulsed Time field, enter the time the pulsed pressure is maintained in the inlet. This field is available only if the Pulsed Split and Pulsed Splitless inlets are selected.

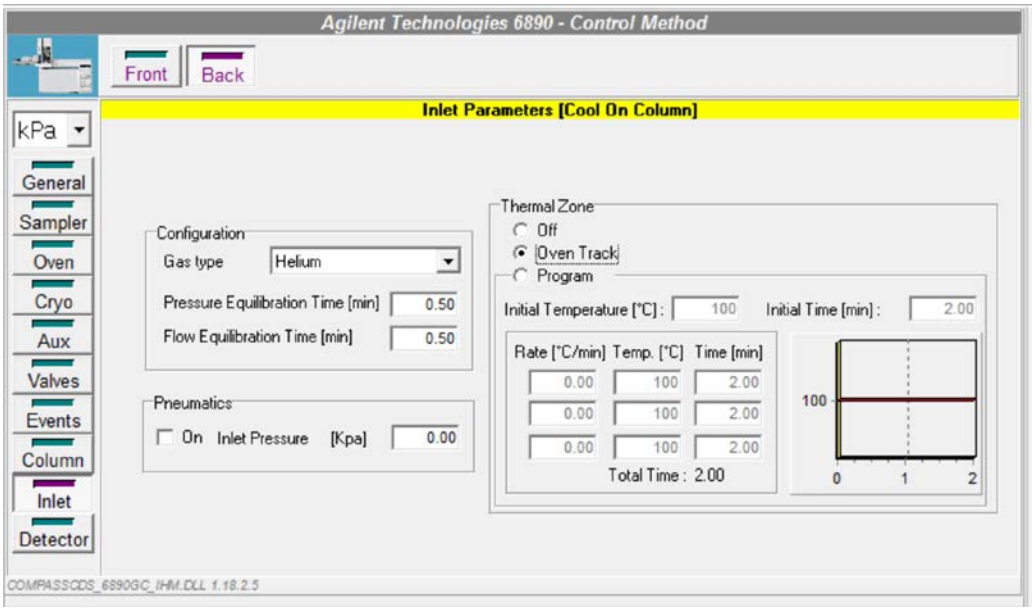
Check the Gas saver on to activate the gas saver. This option is available only if the column parameters have been defined in the Column sub-section.

In the Saver Flow field, enter the gas flow. It must at least equal to column flow, plus 15 mL/min.

In the Saver Time field, enter the time the gas saver is activated. This time must greater than the purge time for splitless injection and greater than injection time for split injection.

NOTE: The Inlet pressure must be equal to the column pressure.

Cool On Column



Configuration Parameter Group

Select the *Gas type*. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, and Unknown.

In the *Pressure Equilibration Time*, enter the time before the inlet pressure becomes ready. In the *Flow Equilibration Time*, enter the time before the inlet flow becomes ready

Pneumatics Parameter Group

Check the *On* box to activate the inlet pressure. Enter the desired pressure.

Thermal Zone Parameter Group

Select the *Off* option to turn off the thermal zone.

Select the *Oven Track* to make the inlet temperature profile track the oven temperature. The difference between the two temperatures is 3°C.

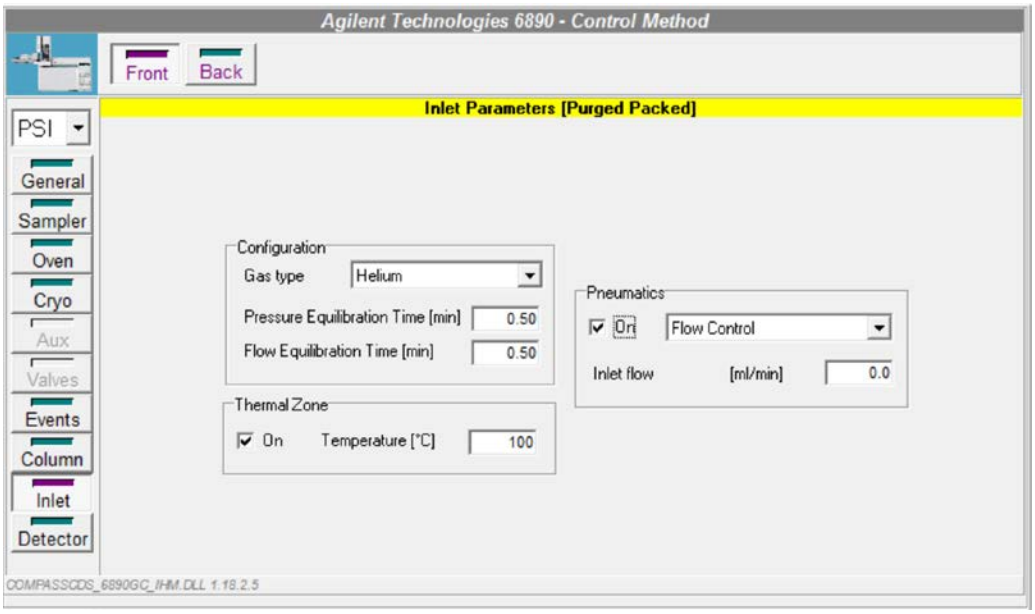
Select *Program* to set the thermal zone program.

In the *Initial Temperature* field, enter the inlet initial temperature in °C.

In the *Initial Time* field, enter the time the inlet stays to the *Initial Temperature* (first plateau) in minutes. In the table program the rates, the plateau temperatures, and duration of the inlet plateau temperature. The graphic on the right of the table displays the temperature program.

The total time of the inlet temperature program is displayed in the *Total Time* field.

Purged Packed



Configuration Parameter Group

Select the *Gas type*. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, and Unknown.

In the *Pressure Equilibration Time*, enter the time before the inlet pressure becomes ready. In the *Flow Equilibration Time*, enter the time before the inlet flow becomes ready.

Thermal Zone Parameter Group

Check the *On* box to activate the inlet temperature. Enter the desired *Temperature*.

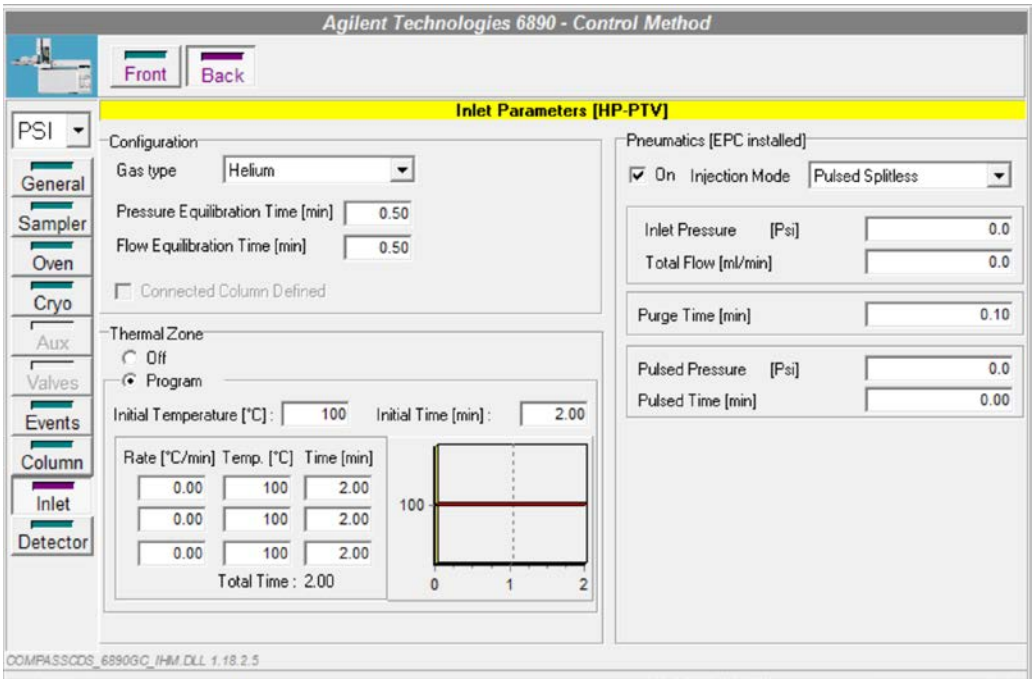
Pneumatics Parameter Group

Check the *On* box to activate the pneumatic parameters.

Select the control mode. The available choices are: *Pressure control* and *Flow control*.

In the *Inlet pressure* field, enter the desired inlet pressure. The unit depends on the control mode choice.

HP – Programmable Temperature Vaporization



Configuration Parameter Group

Select the *Gas type*. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, and Unknown.

In the *Pressure Equilibration Time*, enter the time before the inlet pressure becomes ready. In the *Flow Equilibration Time*, enter the time before the inlet flow becomes ready

The *Connected Column Defined* field is selected if the column configuration has been defined in the *Column* sub- section.

Thermal Zone Parameter Group

Select the *Off* option to turn off the thermal zone. Select *Program* to set the thermal zone program.

In the *Initial Temperature* field, enter the inlet initial temperature in °C.

In the *Initial Time* field, enter the time the inlet stays to the *Initial Temperature* (first plateau) in minutes.

In the table program the rates, the plateau temperatures, and the duration of the inlet plateau temperature. The graphic to the right of the table displays the temperature program.

The total time of the inlet temperature program is displayed in the *Total Time* field.

Pneumatics Parameter Group

Check the *On* box to activate the pneumatic parameters.

Select the *Injection mode*. The available choices are: *Split*, *Splitless*, *Pulsed split*, *Pulsed splitless* and *Solvent Vent*. According to this choice, the following parameters are activated or not.

In the *Inlet Pressure* field, enter the pressure of the inlet.

In the *Split Ratio* field, enter the ratio between the division flow and column flow. This field is available only if the

Split and *Pulsed Split* inlets are selected.

In the *Purge flow* field, enter the flow of the purge vent in mL/min. This field is available only if the *Splitless* and

Pulsed Splitless inlets are selected.

In the *Total Flow* field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined in the *Column* sub-section.

In the *Purge Time field*, enter the time the purge valve is opened. This field is available only if the *Splitless* and *Pulsed Splitless* inlets are selected.

In the *Pulsed Pressure* field, enter the inlet pressure when the acquisition starts. This field is available only if the

Pulsed Split and *Pulsed Splitless* inlets are selected.

In the *Pulsed Time* field, enter the time the pulsed pressure is maintained in the inlet. This field is available only if the

Pulsed Split and *Pulsed Splitless* inlets are selected.

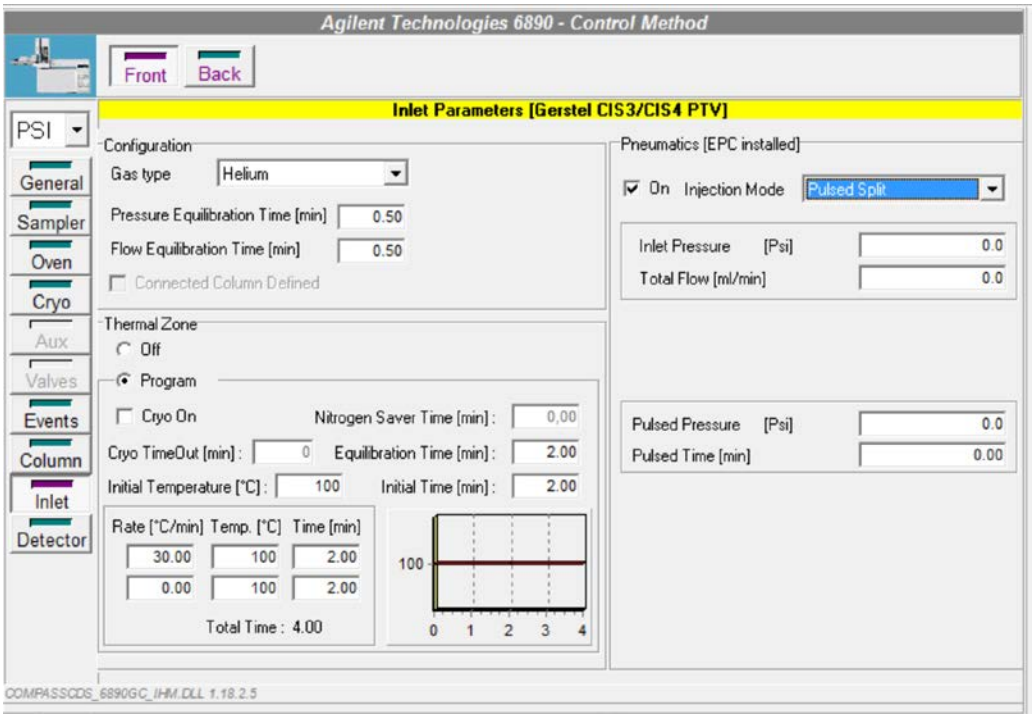
In the *Vent Flow* field, enter the gas flow during the *Vent Time.*

In the *Vent Pressure* field, enter the inlet pressure during the *Vent Time.*

In the *Vent Time* field, enter the vent length from the beginning of the acquisition.

NOTE: The Inlet pressure must be equal to the column pressure.

Gerstel Programmable Temperature Vaporization



Configuration Parameter Group

Select the Gas type. The available choices are: Nitrogen, Hydrogen, Helium and Argon/Methane. In the Pressure Equilibration Time, enter the time before the inlet pressure becomes ready.

In the Flow Equilibration Time, enter the time before the inlet flow becomes ready

The Connected Column Defined field is selected if the column configuration has been defined in the Column sub- section.

Thermal Zone Parameter Group

Select the Off option to turn off the thermal zone. Select Program to set the thermal zone program.

In the Initial Temperature field, enter the inlet initial temperature in °C.

In the Initial Time field, enter the time the inlet stays to the Initial Temperature (first plateau) in minutes.

In the table program the rates, the plateau temperatures, and the duration of the inlet plateau temperature. The graphic to the right of the table displays the temperature program.

The total time of the inlet temperature program is displayed in the Total Time field.

Pneumatics Parameter Group

Check the On box to activate the pneumatic parameters.

Select the Injection mode. The available choices are: Split, Splitless, Pulsed split, Pulsed splitless and Solvent Vent. According to this choice, the following parameters are activated or not.

In the Inlet Pressure field, enter the pressure of the inlet.

In the Split Ratio field, enter the ratio between the division flow and column flow. This field is available only if the Split and Pulsed Split inlets are selected.

In the Purge flow field, enter the flow of the purge vent in mL/min. This field is available only if the Splitless and

Pulsed Splitless inlets are selected.

In the Total Flow field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined in the Column sub-section.

In the Purge Time field, enter the time the purge valve is opened. This field is available only if the Splitless and Pulsed Splitless inlets are selected.

In the Pulsed Pressure field, enter the inlet pressure when the acquisition starts. This field is available only if the

Pulsed Split and Pulsed Splitless inlets are selected.

In the Pulsed Time field, enter the time the pulsed pressure is maintained in the inlet. This field is available only if the

Pulsed Split and Pulsed Splitless inlets are selected.

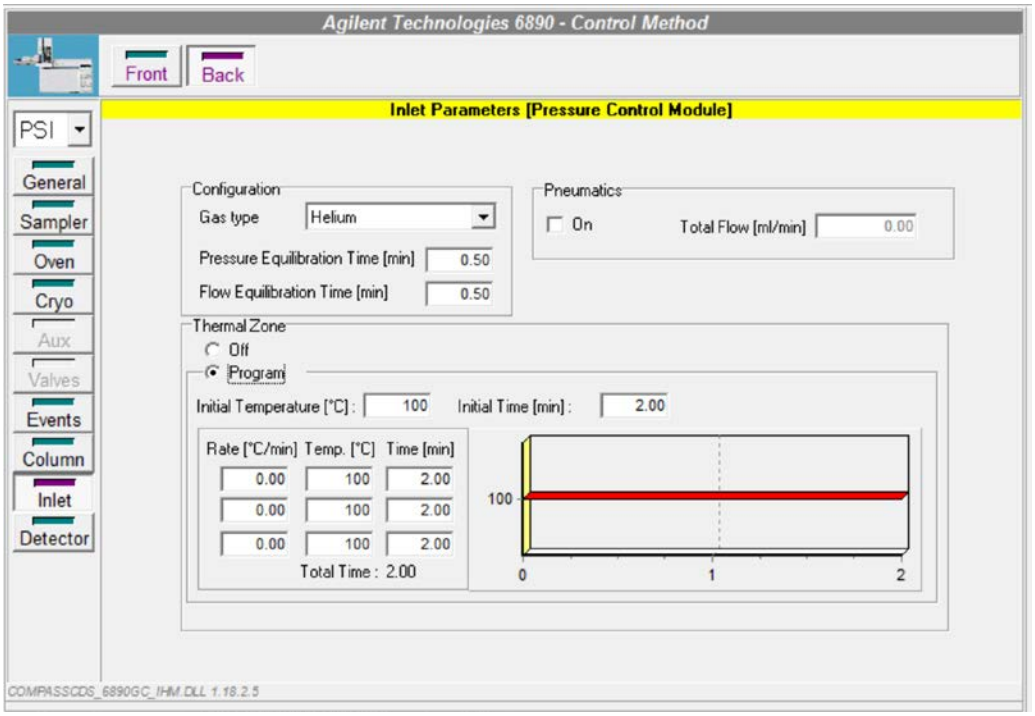
In the Vent Flow field, enter the gas flow during the Vent Time.

In the Vent Pressure field, enter the inlet pressure during the Vent Time.

In the Vent Time field, enter the vent length from the beginning of the acquisition.

NOTE: The Inlet pressure must be equal to the column pressure.

Pressure Control Module (PCM)



Configuration Parameter Group

Select the Gas type. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, Oxygen, Air, Argon, Unknown.

In the Pressure Equilibration Time, enter the time before the inlet pressure becomes ready. In the Flow Equilibration Time, enter the time before the inlet flow becomes ready

Thermal Zone Parameter Group

Check the *On* box to activate the inlet temperature. Enter the desired *Temperature*.

Pneumatics Parameter Group

Check the On box to activate the pneumatic parameters.

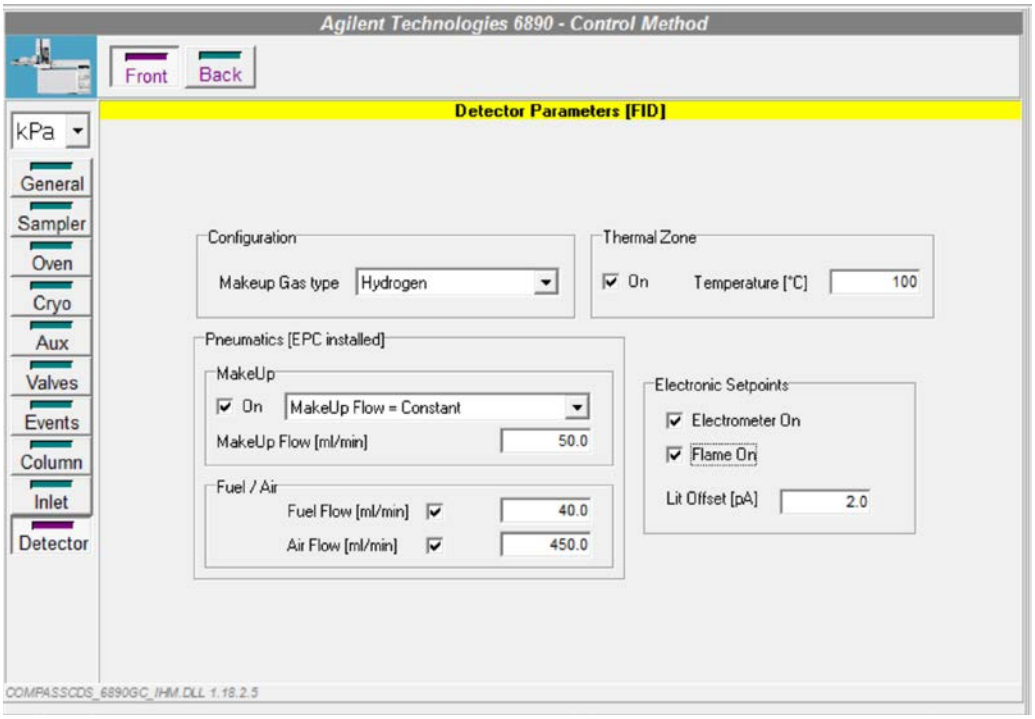
In the Total Flow field, enter the sum of the division flow, the column flow and the septum purge flow.

Detector Control

Depending on the system configuration, select the Front or Back button, to set the information for each detector. The different fields depend on system configuration.

NOTE: The Agilent Technologies 6850 Gas Chromatograph has only one sub-system. Therefore, only the *Front* information must be set.

FID (Flame Ionization Detector)



Configuration Parameter Group

Select the *Makeup Gas type*. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, and Unknown.

Pneumatics Parameter Group

Check the *On* box to force a constant flow.

Select if either the *MakeUp Flow* or the *MakeUp Flow + Column Flow* must be constant. Enter the corresponding constant flow in mL/min

In the *Fuel Flow* field, enter the detector gas flow (typically, hydrogen). In the *Air Flow* field, enter the detector air flow.

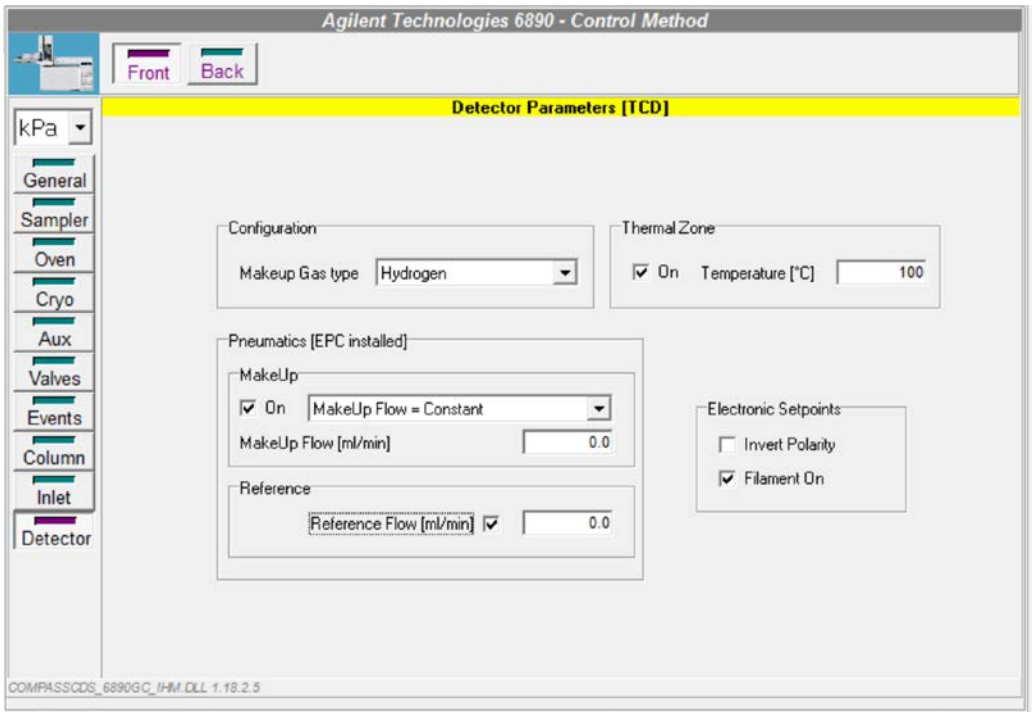
Thermal Zone Parameter Group

Check the *On* box to turn on the detector heater. Enter the desired *Temperature*. Electronic Setpoints parameter group

Check the *Electrometer On* box to turn on the electrometer. Check the *Flame On* box to ignite the flame.

Optionally, enter a *Lit Offset*. This value is the difference between the output when the flame is on and the output when the flame is off. Default value is 2pA.

TCD (Thermal Conductivity Detector)



Configuration Parameter Group

Select the Makeup Gas type. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, and Unknown.

Pneumatics Parameter Group

Check the *On* box to force a constant flow.

Select if either the *MakeUp Flow* or the *MakeUp Flow + Column Flow* must be constant. Enter the corresponding constant flow in mL/min.

Check the *Reference Flow* box and enter the reference gas flow in mL/min.

Thermal Zone Parameter Group

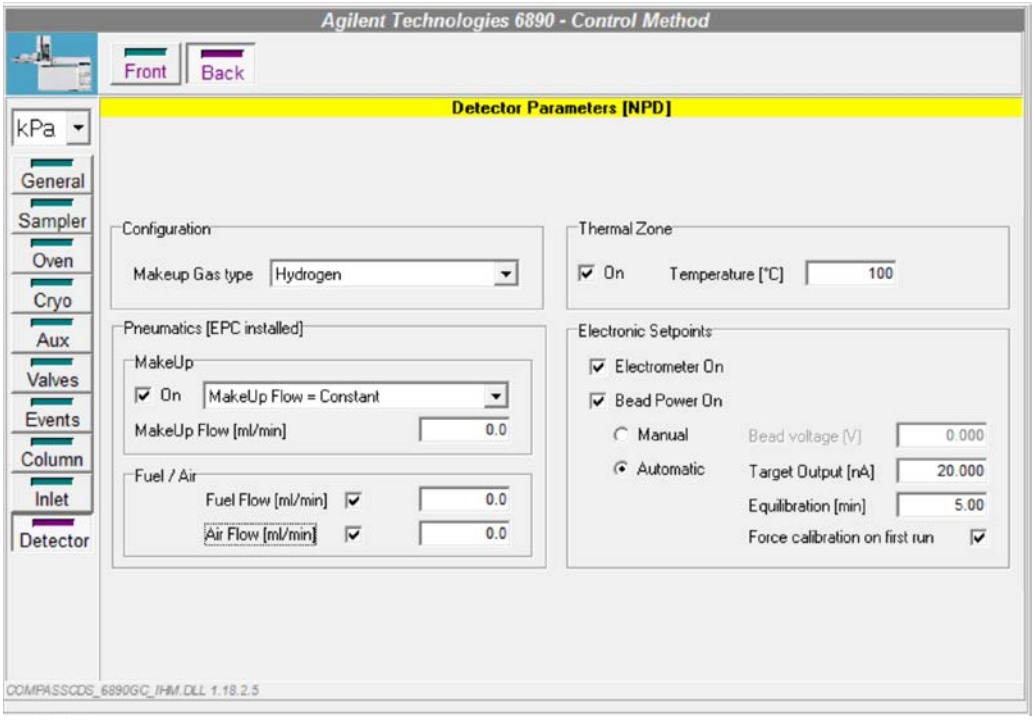
Check the *On* box to turn on the detector heater. Enter the desired *Temperature*.

Electronic Setpoints Parameter Group

Check the *Invert polarity* box to invert the filament polarity. This option must be activated when the thermal conductivity of the components is greater than the carrier gas, otherwise the peaks will be negative.

Check the *Filament On* box to turn on the voltage to the filament.

NPD (Nitrogen-Phosphorus Detector)



Configuration Parameter Group

Select the *Makeup Gas type*. The available choices are: Nitrogen, Hydrogen, Helium, Argon/Methane, and Unknown.

Pneumatics Parameter Group

Check the *On* box to force a constant flow.

Select if either the *MakeUp Flow* or the *MakeUp Flow + Column Flow* must be constant. Enter the corresponding constant flow in mL/min

In the *Fuel Flow* field, enter the detector gas flow (typically, hydrogen). In the *Air Flow* field, enter the detector air flow.

Thermal Zone Parameter Group

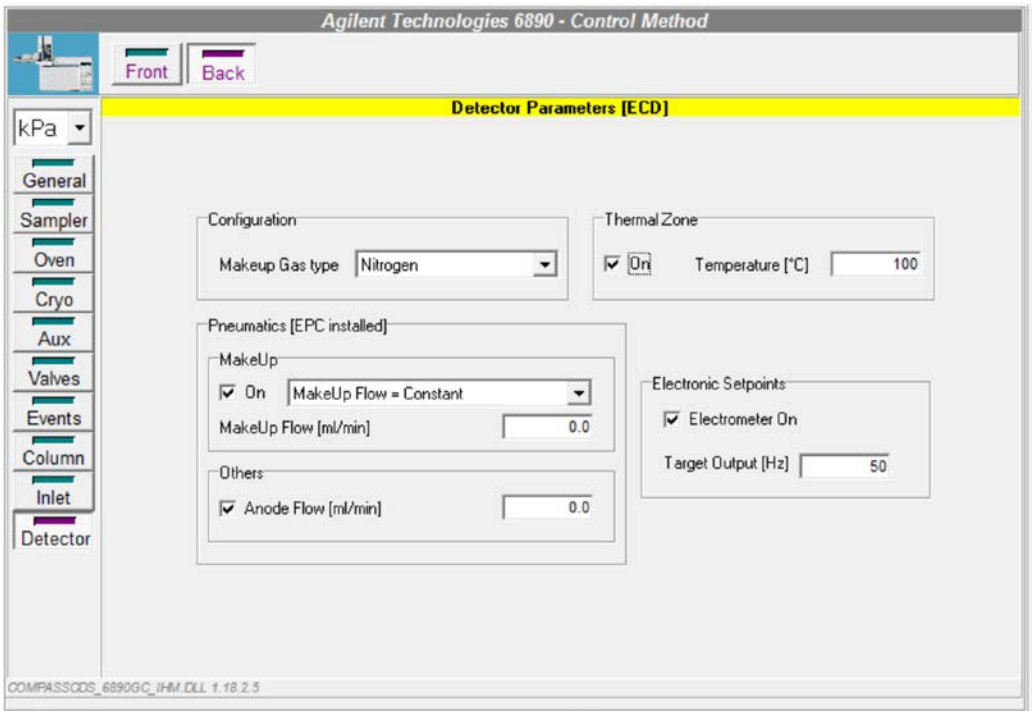
Check the *On* box to turn on the detector heater. Enter the desired *Temperature*.

Electronic Setpoints Parameter Group

Check the *Electrometer On* box to turn on the electrometer. Check the *Bead Power On* box to heat the bead.

- Select *manual* to enter the *Bead voltage* use to heat the bead.
- Select *Automatic* and fill the *Target Output [nA]*, the time of *Equilibration [min*] and if you want or not *Force calibration on first run*

ECD (Electron Capture Detector)



Configuration Parameter Group

Select the Makeup Gas type. The available choices are: Nitrogen, Argon/Methane, and Unknown.

Pneumatics Parameter Group

Check the *On* box to force a constant flow.

Select if either the *MakeUp Flow* or the *MakeUp Flow + Column Flow* must be constant. Enter the corresponding constant flow in mL/min

In the *Anode Flow* field, enter the anode gas flow.

Thermal Zone Parameter Group

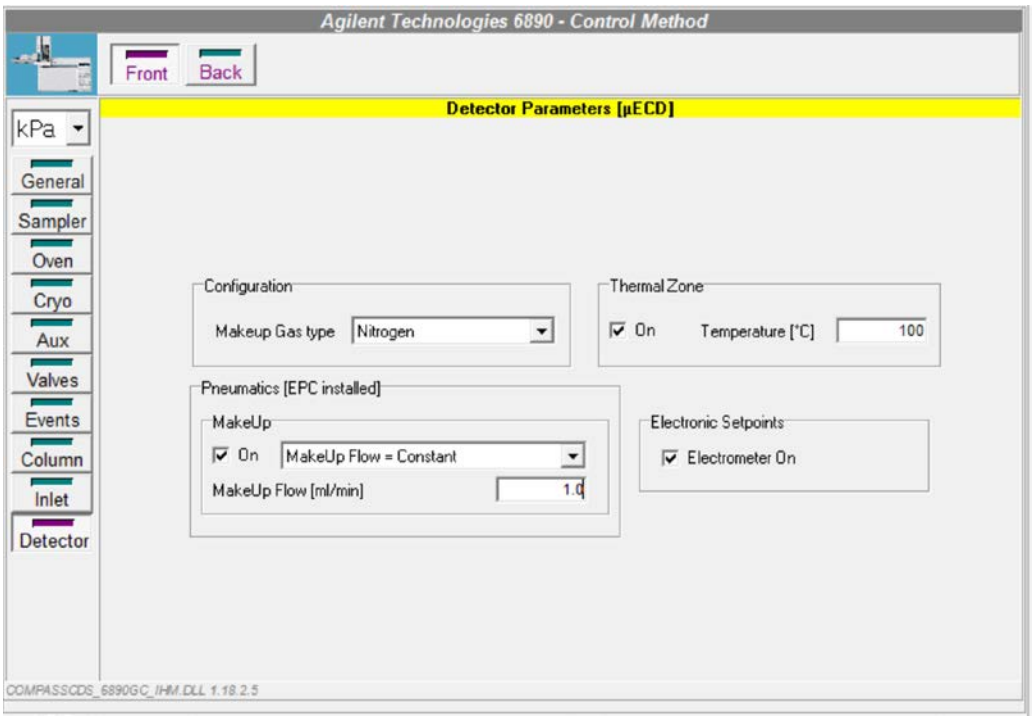
Check the On box to turn on the detector heater. Enter the desired Temperature.

Electronic Setpoints Parameter Group

Check the *Electrometer On* box to turn on the electrometer.

In the *Target Output* field, enter the detector target output in Hz.

µECD (micro Electron Capture Detector)



Configuration Parameter Group

Select the Makeup Gas type. The available choices are: Nitrogen, Argon/Methane, and Unknown.

Pneumatics Parameter Group

Check the *On* box to force a constant flow.

Select if either the *MakeUp Flow* or the *MakeUp Flow + Column Flow* must be constant. Enter the corresponding constant flow in mL/min

Thermal Zone Parameter Group

Check the On box to turn on the detector heater. Enter the desired Temperature.

Electronic Setpoints Parameter Group

Check the *Electrometer On* box to turn on the electrometer.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

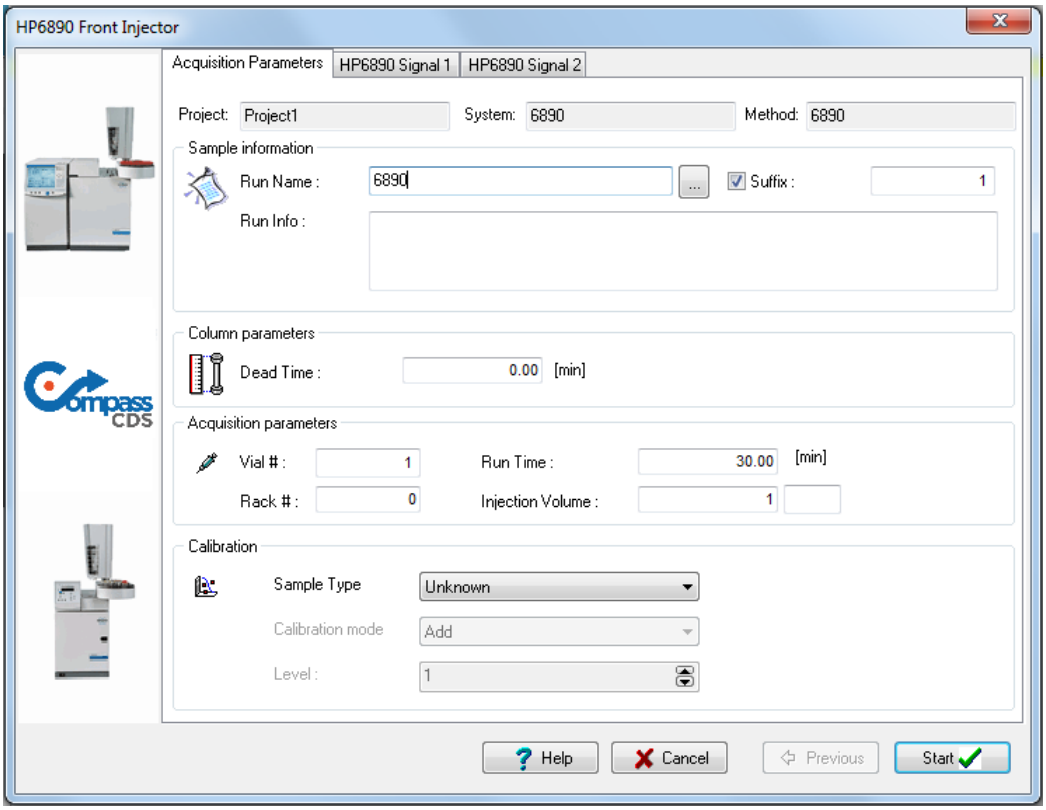
Quick Start (Single Acquisition)

1. Press the button.

   In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

2. Press the OK button.

   The following screen is displayed



   In the Acquisition parameters tab, required fields like the Run Name, the Run ID and the Acquisition length must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the Injection Volume, the Vial position and the Rack number (if required) must be entered.

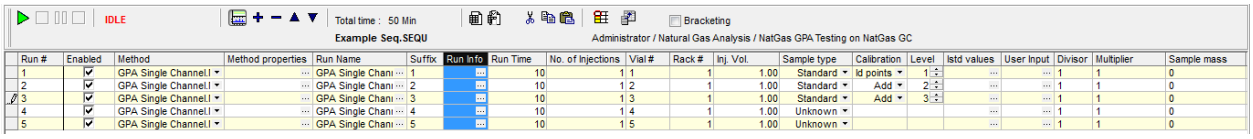
   Other parameters associated with each acquisition channel can be entered in the Channel X tab.

3. Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector

system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

1. To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data System User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.
2. The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS Chromatography Data System User Guide).



Run #	Enabled	Method	Method properties	Run Name	Suffix	Run Info	Run Time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type	Calibration	Level	Istd values	User Input	Divisor	Multiplier	Sample mass
1	☑	GPA Single Channel.I		GPA Single Chani	1		10	1	1	1	1.00	Standard	Id points	1			1	1	0
2	☑	GPA Single Channel.I		GPA Single Chani	2		10	1	2	1	1.00	Standard	Add	2			1	1	0
3	☑	GPA Single Channel.I		GPA Single Chani	3		10	1	3	1	1.00	Standard	Add	3			1	1	0
4	☑	GPA Single Channel.I		GPA Single Chani	4		10	1	4	1	1.00	Unknown					1	1	0
5	☑	GPA Single Channel.I		GPA Single Chani	5		10	1	5	1	1.00	Unknown					1	1	0

The Method Name, the Run Name, the Run ID, and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

3. Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS Chromatography Data System User Guide.

NOTE: The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for this driver in the Acquisition sub-method part: 1, 2, 3, 4 and 5. These values represent the number of tenths of the syringe volume. For example if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 tenths of 10 µL=3 µL. A physical turret option called Nanoliter allows the injection of smaller volume (refer to the Agilent manual to learn more about this option). Refer to the Appendix (Injection Volumes section) to see the correspondence between the programmed levels and the real injected volumes.

Running Acquisition Status

Viewing a Running Acquisition

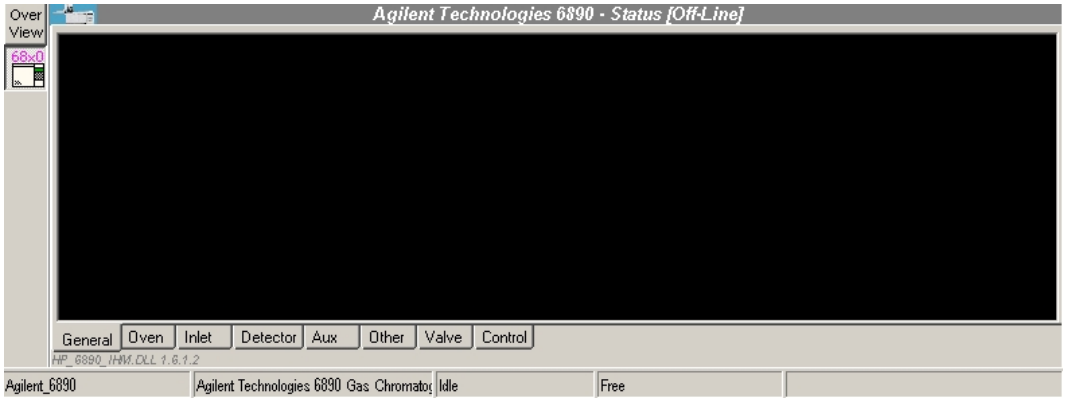
To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Agilent 6890 Gas Chromatograph

Click on the button corresponding to the Agilent 6890 Gas Chromatograph driver and the Agilent Technologies 6890 Gas Chromatograph status screen will appear. It contains nine sub-sections: General, Oven, Inlet, Detector, Aux, Other, Valve, Control and, Gerstel. Click on the required sub-section to display the corresponding screen.

Click on the correct node in the tree-view to display the corresponding screen.

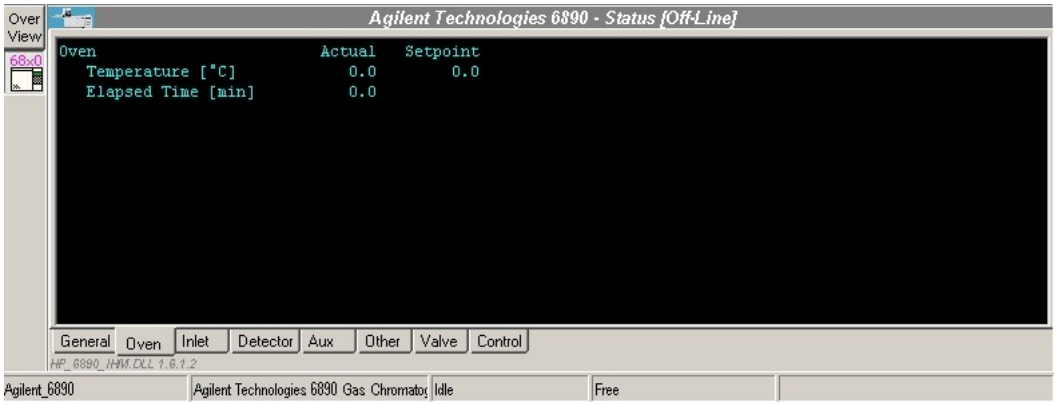
General Window



This is a read-only window.

Information about the instrument status is displayed: Faults, not ready parameters, etc.

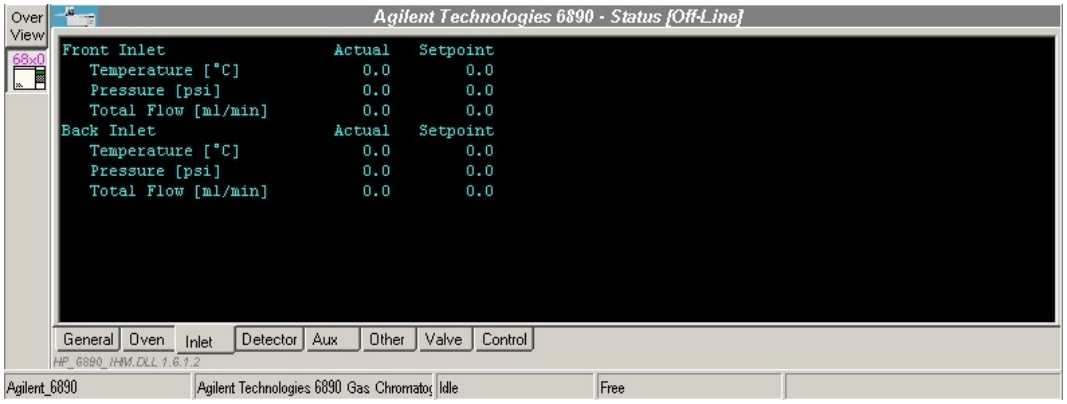
Oven Window



This is a read-only window.

The actual and setpoint temperatures of the oven and the elapsed time are displayed.

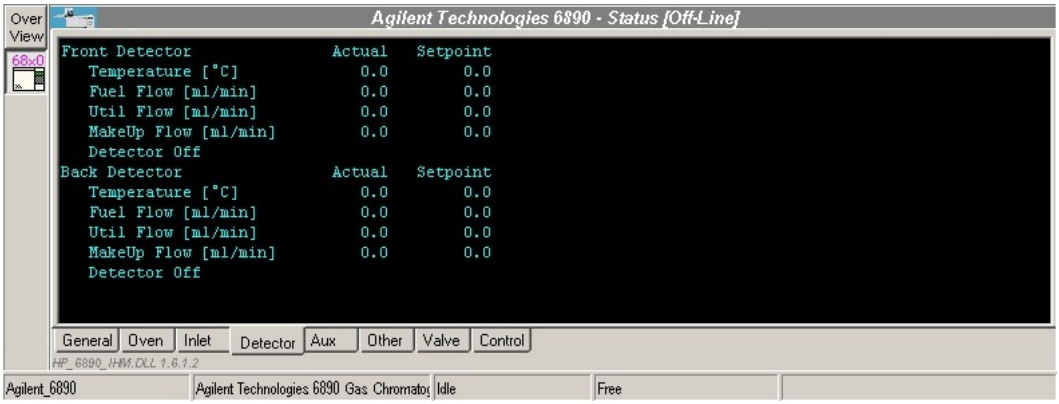
Inlet Window



This is a read-only window.

The actual and setpoint temperature, pressure, and flow of the inlet(s) are displayed.

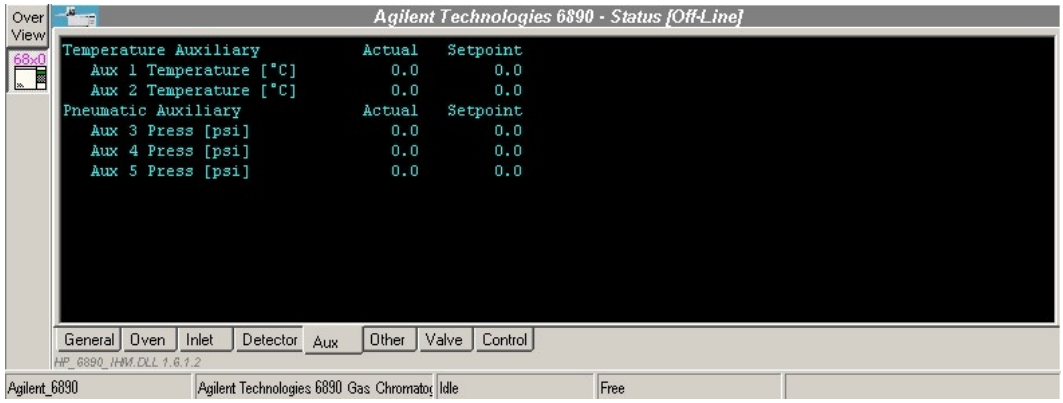
Detector Window



This is a read-only window.

The actual and setpoint temperatures and gas flows of the detector(s) are displayed.

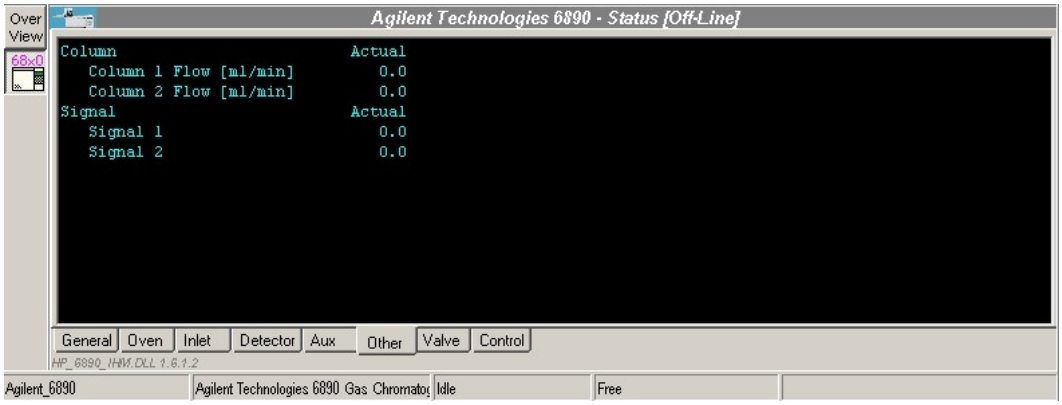
Aux Window


Agilent Technologies 6890 - Status [Off-Line]
Temperature Auxiliary Actual Setpoint
Aux 1 Temperature [°C] 0.0 0.0
Aux 2 Temperature [°C] 0.0 0.0
Pneumatic Auxiliary Actual Setpoint
Aux 3 Press [psi] 0.0 0.0
Aux 4 Press [psi] 0.0 0.0
Aux 5 Press [psi] 0.0 0.0
General Oven Inlet Detector Aux Other Valve Control
Agilent_6890
Idle
Free

This is a read-only window.

The actual and setpoint temperatures or pressures of the auxiliary(ies) are displayed.

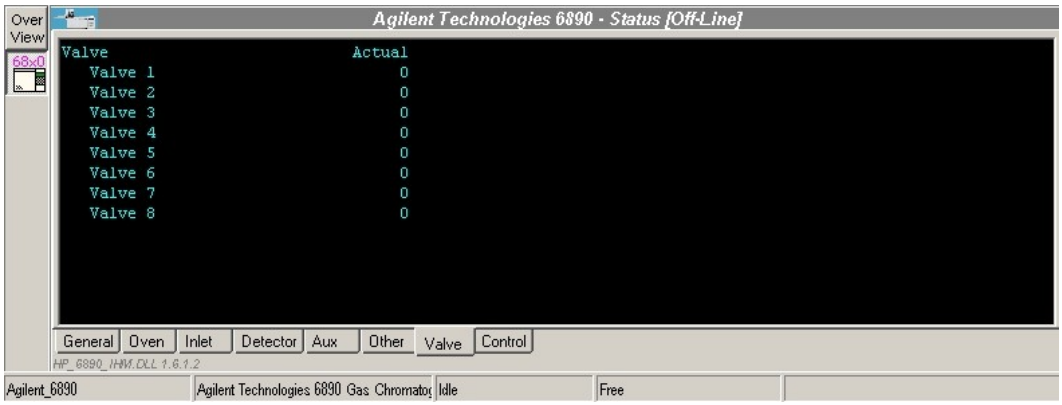
Other Window



This is a read-only window.

The actual column flows are displayed.

Valve Window



This is a read-only window.

The actual valve positions are displayed.

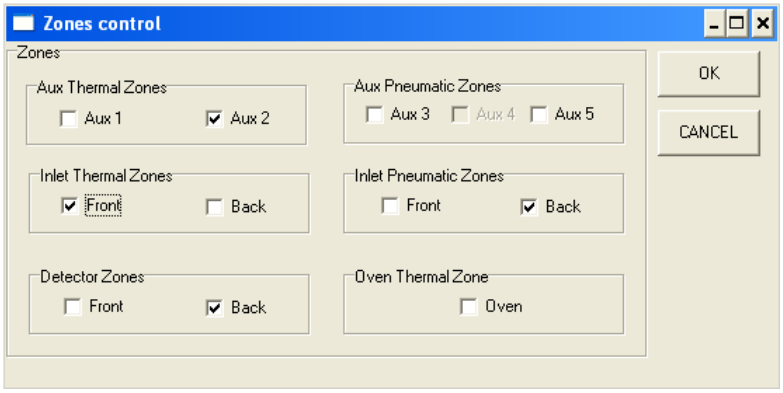
Control Window

This window allows direct control of the 6890 GC.

unlocks the chromatograph keyboard

locks chromatograph keyboard

gives access to the Zone control screen



From this screen, you can turn on/off the different thermal zones of the GC.

The button stops the chromatograph.

Select *Set Oven Temperature* line, to change the oven temperature and then enter the desired temperature in the

Oven Temperature field and click on the button to send the new value to the 6890 GC.

Select *Set front (*or *Back) Detector Temperature* line, to change the detector temperature and then enter the desired temperature in the *front (*or *Back) Detector Temperature* field and click on the button to send the new value to the 6890 GC.

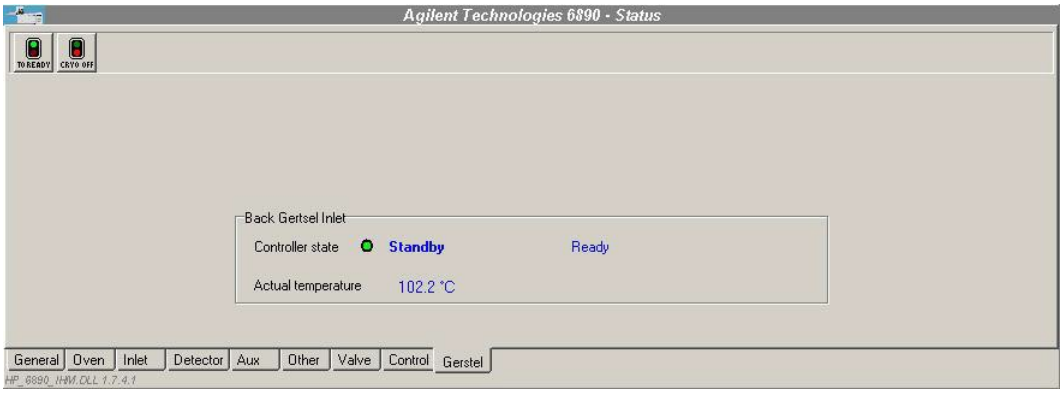
Select *Set front (*or *Back) Inlet Temperature* line, to change the inlet temperature and then enter the desired temperature in the *front (*or *Back) Inlet Temperature* field and click on the button to send the new value to the 6890 GC.

Select *Set Aux1 (*or *Aux2) Temperature* line, to change the auxiliary temperature and then enter the desired temperature in the *Aux1 (*or *Aux2) Temperature* field and click on the button to send the new value to the 6890 GC.

NOTE: Each time a method is downloaded to the instrument, the flow rate is updated to the value in the method and the flow rate sent with the direct control window is overwritten.

NOTE: All the direct control buttons are deactivated during a run.

Gerstel Window



This is a read-only window.

The state and the temperature of the Gerstel PTV are displayed.

turns on the cryogenic cooling of the Gerstel PTV

turns off the cryogenic cooling of the Gerstel PTV

Overview Window

Click on the

button: for 6890 GC, nothing is displayed.

Appendix

Injection Volumes

The volume that will be injected depends of the syringe size. Only five levels of injection volume can be programmed for the 6890 in the Acquisition sub-method part: 1, 2, 3, 4 and 5, and six levels of injection volume can be programmed for the 6850 in the Acquisition sub-method part: 1, 2, 3, 4, 5 and 6. These values represent the number of tenths of the syringe volume. For example if the entered volume is 3 and the syringe volume is 10 µL, the injected volume will be 3 tenths of 10 µL = 3 µL. A physical turret option called *Nanoliter* allows the injection of smaller volume (refer to the Agilent manual to learn more about this option). The following table gives the injected volumes according to the value entered in the Acquisition sub-method part.

Injection volume depending on the syringe volume for the 6890

Nanoliter Option	Off - 6890		On - 6890	
	Entered Value	**Injected Volume**	**Entered Value**	**Injected Volume**
5 µL Syringe	1	0.5	1	0.1
	2	1.0	2	0.5
	3	1.5	3	1.0
	4	2.0	4	1.5
	5	2.5	5	2.0
10 µL Syringe	1	1.0	1	0.2
	2	2.0	2	1.0
	3	3.0	3	2.0
	4	4.0	4	3.0
	5	5.0	5	4.0
25 µL Syringe	1	2.5	1	0.5
	2	5.0	2	2.5
	3	7.5	3	5.0
	4	10.0	4	7.5
	5	12.5	5	10.0
50 µL Syringe	1	5.0	1	1.0
	2	10.0	2	5.0
	3	15.0	3	10.0
	4	20.0	4	15.0
	5	25.0	5	20.0
100 µL Syringe	1	10.0	1	2.0
	2	20.0	2	10.0
	3	30.0	3	20.0
	4	40.0	4	30.0
	5	50.0	5	40.0

Injection volume depending on the syringe volume for the 6850

Nanoliter Option	Off - 6850		On - 6850	
	Entered Value	**Injected Volume**	**Entered Value**	**Injected Volume**
5 µL Syringe	1	0.5	1	0.1
	2	1.0	2	0.5
	3	1.5	3	1.0
	4	2.0	4	1.5
	5	2.5	5	2.0
			6	2.5
10 µL Syringe	1	1.0	1	0.2
	2	2.0	2	1.0
	3	3.0	3	2.0
	4	4.0	4	3.0
	5	5.0	5	4.0
			6	5.0
25 µL Syringe	1	2.5	1	0.5
	2	5.0	2	2.5
	3	7.5	3	5.0
	4	10.0	4	7.5
	5	12.5	5	10.0
			6	12.5
50 µL Syringe	1	5.0	1	1.0
	2	10.0	2	5.0
	3	15.0	3	10.0
	4	20.0	4	15.0
	5	25.0	5	20.0
			6	25.0
100 µL Syringe	1	10.0	1	2.0
	2	20.0	2	10.0
	3	30.0	3	20.0
	4	40.0	4	30.0
	5	50.0	5	40.0
			6	50.0

Configuring the GC RS232 Communication

This appendix describes how to fix the IP address in the Agilent 6890 GC.

1. On the GC, press the [OPTION] button. The following screen will be displayed.

2. Scroll down to the Communication line and press [ENTER]. The following screen will be displayed.

3. Scroll down to the Baud rate line and press the [MODE/TYPE] button.

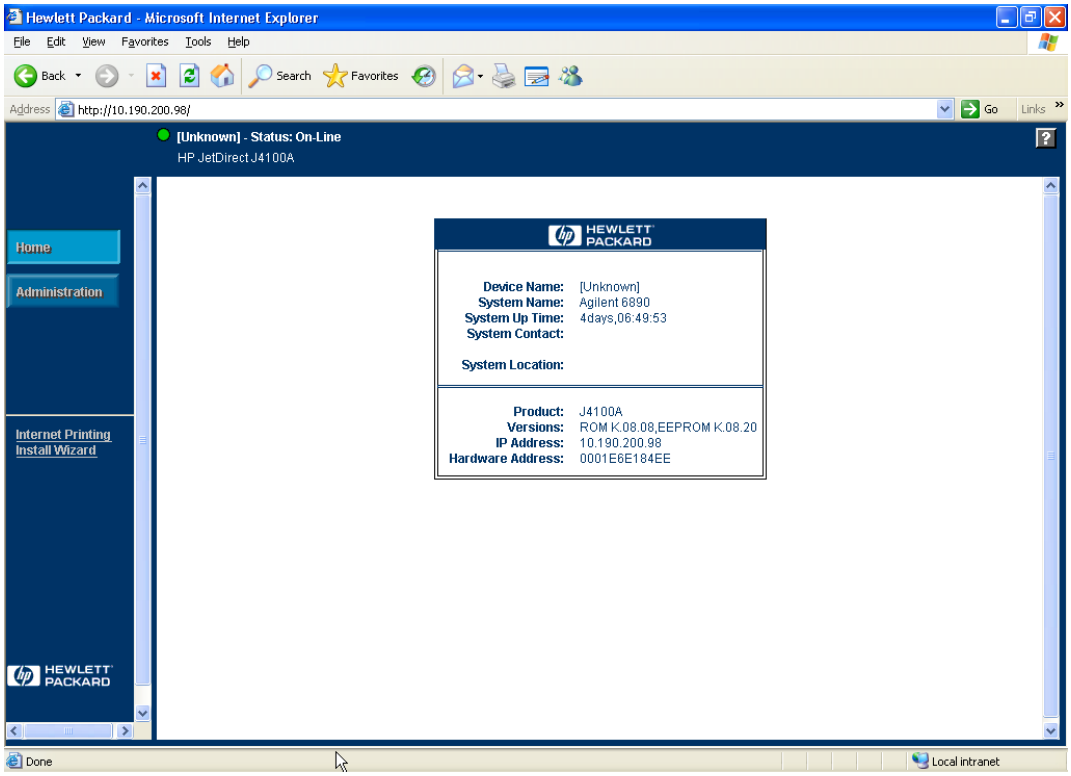
4. Scroll down the arrow to the 19200 line and press [ENTER].
5. Repeat the same operation for the rest of the parameters until all the parameters are set like below.

6. Reboot the GC.

Configuring a Fixed IP address

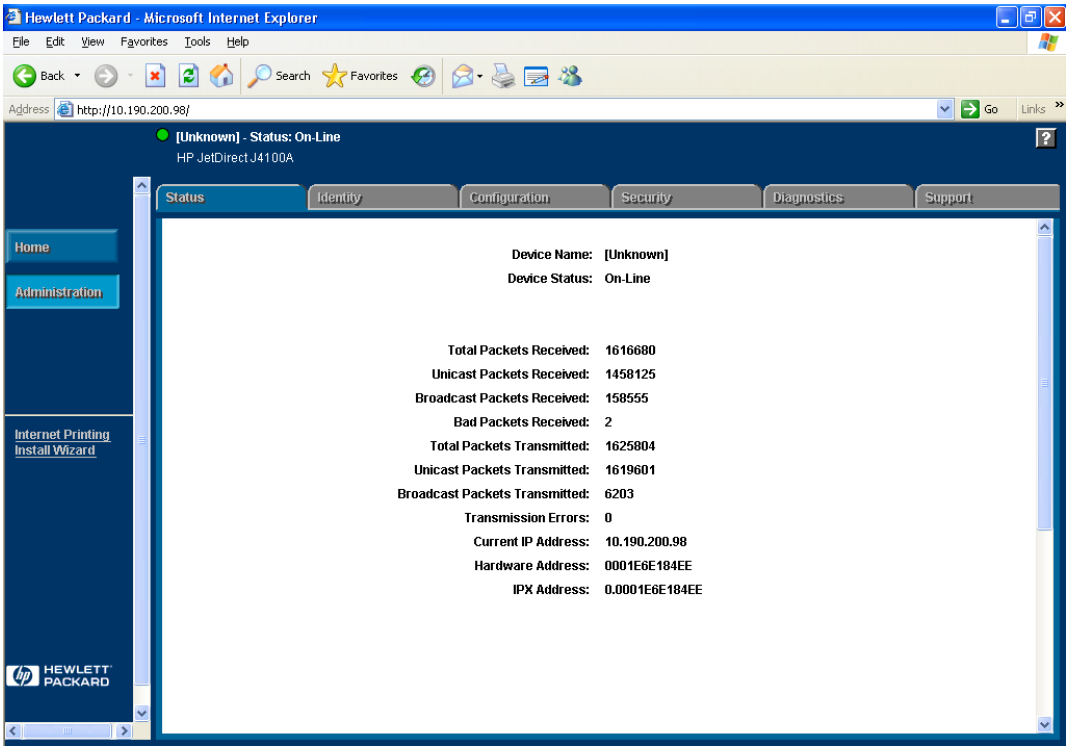
This appendix describes how to fix the IP address in the Agilent 6890 GC.

1. The Agilent 6890 GC must have been given a valid IP address via the BOOTP server.
2. In a web browser (Internet explorer for example) from the Acquisition server, type the IP address of the GC, in the address field. If the Internet browser is configured with a proxy server, it is mandatory to enter the IP address of the GC in the exceptions list. The following screen will be displayed.

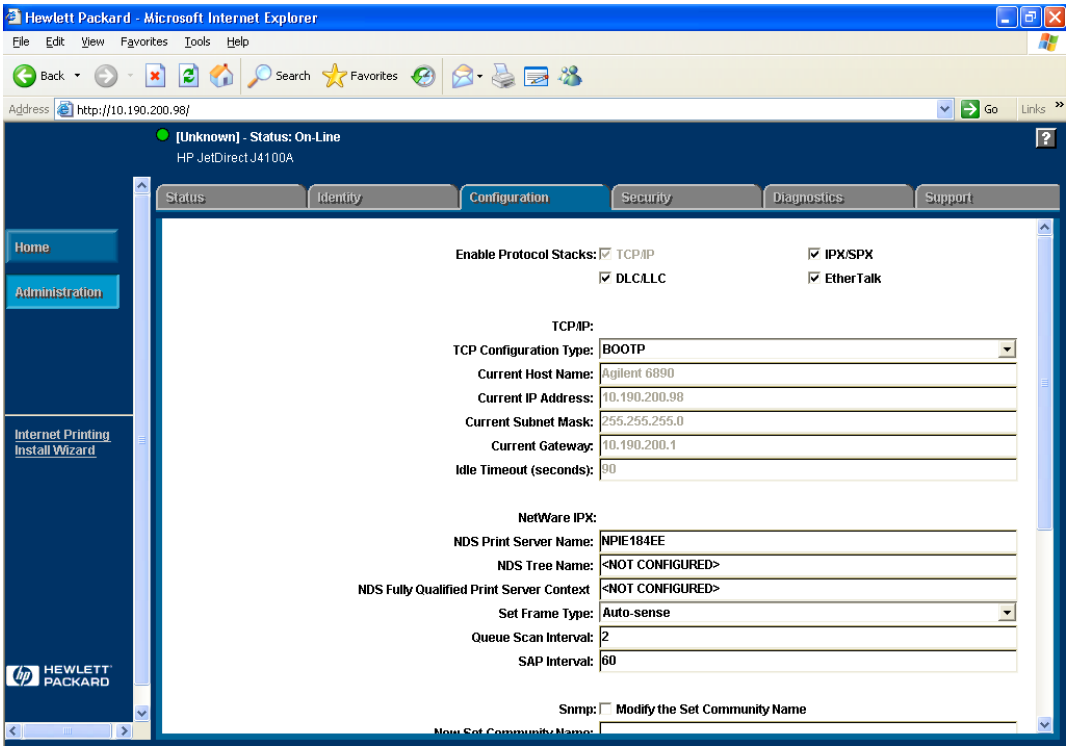


3. Click on the

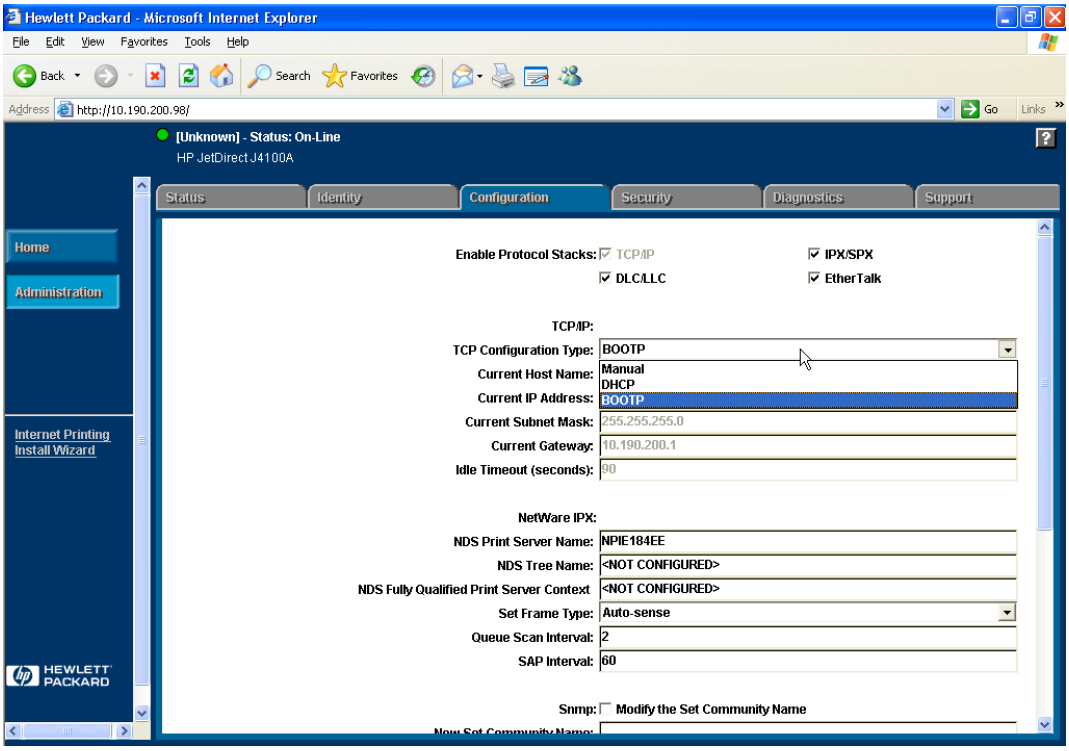
button on the left of the screen.



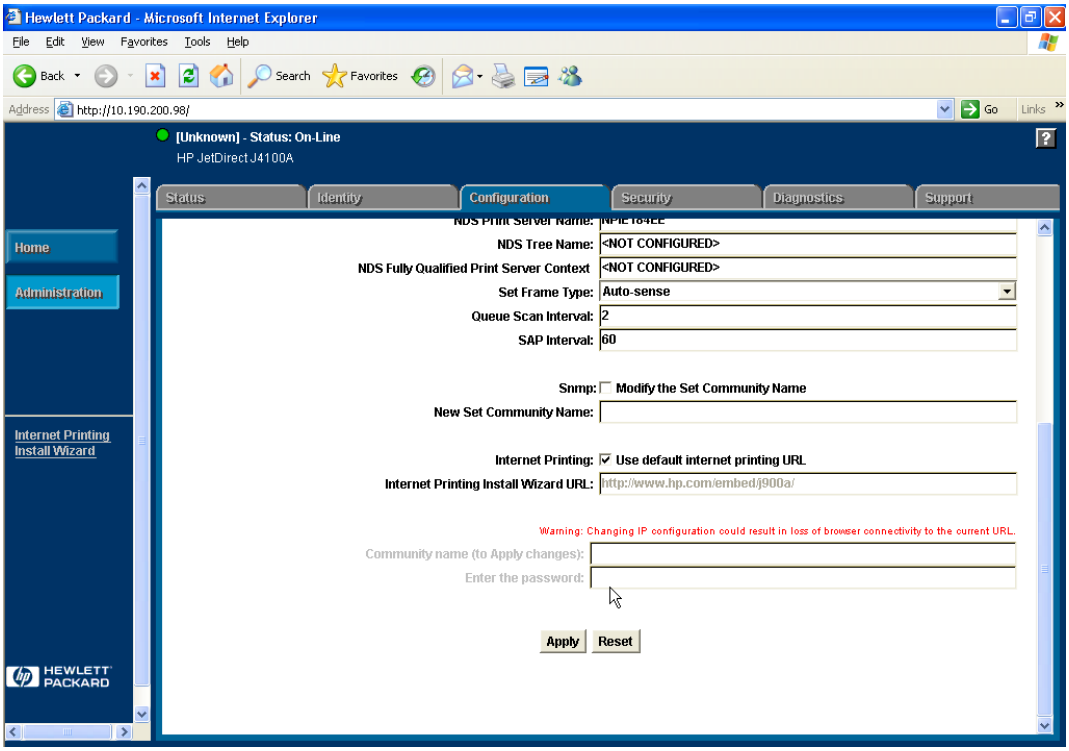
4. Click on the Configuration tab.



5. Select Manual in the *TCP Configuration Type* dropdown list.



6. Type the desired IP address, subnet mask and gateway in the corresponding fields.
7. Finally, scroll down to the bottom of the screen and press the Apply button.


Hewlett Packard - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites
Address http://10.190.200.98/
Go Links
[Unknown] - Status: On-Line
HP JetDirect J4100A
Status Identity Configuration Security Diagnostics Support
Home
Administration
Internet Printing Install Wizard
HEWLETT PACKARD
NDS Tree Name: <NOT CONFIGURED>
NDS Fully Qualified Print Server Context <NOT CONFIGURED>
Set Frame Type: Auto-sense
Queue Scan Interval: 2
SAP Interval: 60
Snmp: Modify the Set Community Name
New Set Community Name:
Internet Printing: Use default internet printing URL
Internet Printing Install Wizard URL: http://www.hp.com/embed/j900a/
Warning: Changing IP configuration could result in loss of browser connectivity to the current URL.
Community name (to Apply changes):
Enter the password:
Apply Reset

8. Reboot the GC.

Agilent 6890 & 6850 GC Control Driver Release Notes

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501585
Revision C

Introduction of the driver (4.0.0)

The Agilent 6890 & 6850 GC CompassCDS control driver software needs CompassCDS version 3.0.1 or above (the CompassCDS versions 2.0 and 3.0 are not supported).

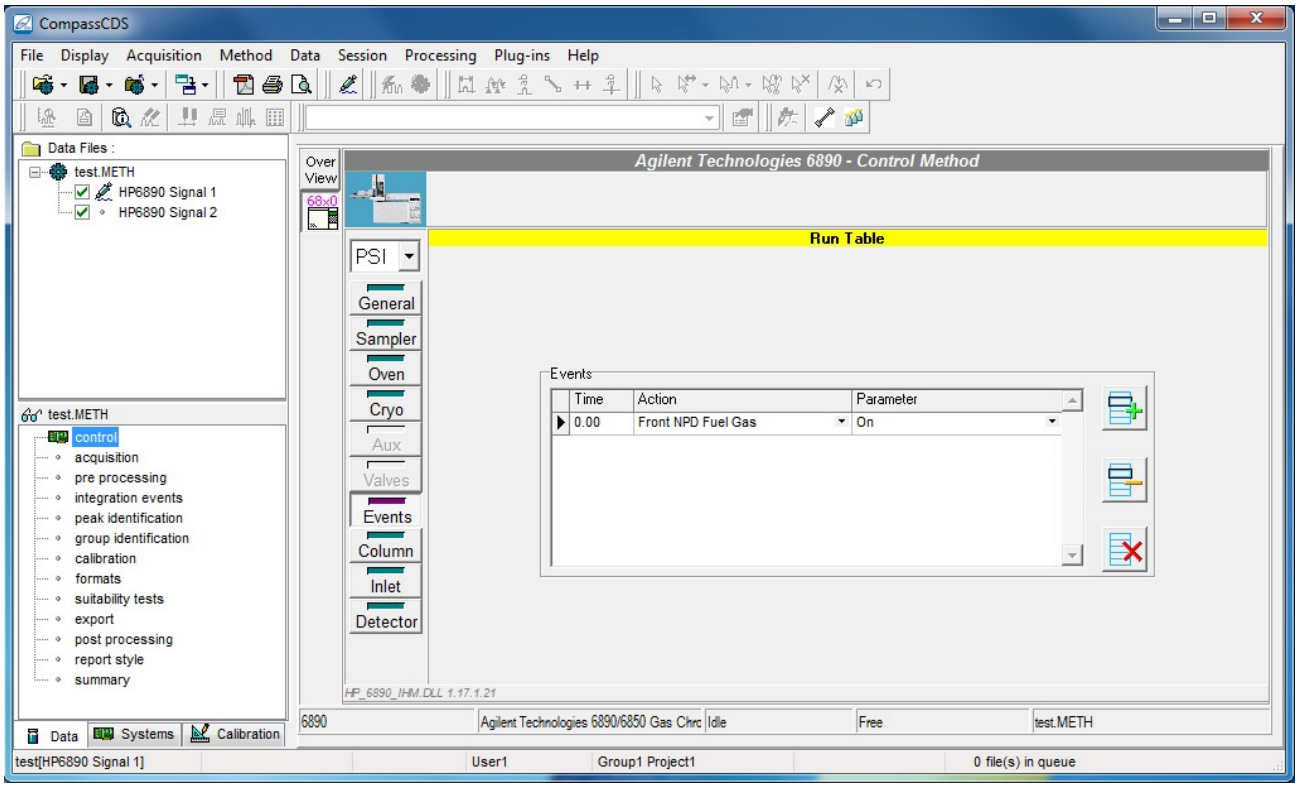
The Agilent 6890 GC can be controlled by CompassCDS software if the GC has the firmware version A.03.08 or above. RS-232 control of older 6890 models via a PC COM port or STAR 800 & 850 MIB serial ports is possible however the latter requires the CompassCDS STAR 800 & 850 MIB control driver (BR502064). The majority of 6890 & 6850 units are controlled via Ethernet.

Supported configurations

- Inlets:
    - Split/splitless capillary inlet (S/SL)
    - Temperature-programmable cool on-column inlet (PCOC)
    - Purge Packed inlet (PP)
    - Gerstel CIS3 and CIS4 Programmable temperature vaporization (PTV)
    - HP-Programmable temperature vaporization (HP-PTV)
- Detectors:
    - Flame ionization detector (FID)
    - Thermal conductivity detector (TCD)
    - Electron capture detector (ECD) and µECD
    - Nitrogen Phosphorous detector (NPD)
- Autosampler: Automatic liquid sampler (ALS) type 7683 (G2913A and G2613A) including the 100 vials tray (G2614A), type 7693A (G4513A) including the 150 vials tray (G4514A), type 7673 (G1513A) including the 100 vials tray (18596A) and the controller module (G1512A).
- The Oven Cryogenic coolant is controlled
- PCM (Pressure Control Module) is controlled
- Multi injector, multi detector: CompassCDS can control any 2 auto sampler, 2 Inlet, 2 detector configuration as long as the configuration consists of the elements described above.
- Valves. Eight valves can be controlled. Among them we support the Gas Sampling valve, the Switching valve and the Multi-position valve.
- Two auxiliary heaters can be controlled.
- Three Auxiliary EPCs can be controlled
- Run time events.

Known issues

- The configuration of the system cannot be printed.
- The two run table events “**NPD Fuel Gas On**” and “**NPD Fuel Gas Off**” have not been validated on 6890 NPD hardware. As consequence, we recommend to not use these run table events. Please contact your local service representative if you need to use this capability.



Agilent 7890 GC Control Driver User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501553
Revision C

Contents

Introduction 3
Installation and Configuration 3
Installing the Driver Software 3
Configuring the GC Communications 3
Ethernet Communications 3
Configuring the Driver 3
Configuring the Agilent 7890 Gas Chromatograph 3
Communication Window 4
Autosampler Window 4
Inlets Window 5
Columns Window 5
Oven Window 5
Valves Options Window 6
Auxiliary Options Window 6
Auxiliary EPC Options Window 6
Pressure Control Module Options Window 7
Detectors Window 7
Building a Method 8
Creating a New Method 8
Control Method Section for the Agilent 7890 Gas Chromatograph 10
Autosampler Control 11
Inlet Control 16
Column Control 21
Oven Control 23
Valves Control 23
Auxiliary heaters Control 25
Pressure Control Module 25
Auxiliary Pressure Control 26
Detector Control 27
Events Control 30
General Control 31
Starting and Viewing an Acquisition 32
Quick Start and Sequence 32
Quick Start (Single Acquisition) 32
Sequence 33
Running Acquisition Status 33
Viewing a Running Acquisition 33
Status of the Agilent 7890 Gas Chromatograph 33
Overview Window 41
Troubleshooting 41
Error message when downloading a method 41
Appendix 42
Injection Volumes 42
7683 autosampler model (G2613, G2913 turret) 42
7693 autosampler model (G4513 turret) 43
GC error codes 43
Autosampler error codes 44

Introduction

This document describes the configuration of the Agilent 7890 Gas Chromatograph driver. It also explains how to build a control method for this driver, how to start and view a running acquisition and which actions are available during an analysis.

Installation and Configuration

Installing the Driver Software

To install the CompassCDS Drivers software, refer to the CompassCDS installation Guide.

Configuring the GC Communications

Ethernet Communications

The Agilent 7890 Gas Chromatograph uses Ethernet® as the method of communications for instrument control and for sending digital data to the external data system.

Ethernet communication is standard on the Agilent 7890 GC.

The Ethernet connection is made at the back at the 7890 GC. There are two types of Ethernet cables:

- An Ethernet crossover cable is used when the Agilent 7890 GC is connected directly to the CompassCDS Acquisition Server PC.
- A standard Ethernet patch cable is used when the Agilent 7890 GC is connected to a company Ethernet network.

The Agilent 7890 GC uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server or a DHCP server is used to send IP addresses to TCP/IP devices.

The BOOTP Server lists Ethernet addresses along with the IP addresses that are to be assigned to the corresponding devices.

To know how to configure the BOOTP server, refer to the CompassCDS Installation Guide.

It is also possible to give a fixed IP address to the GC. To know how to fix the IP address of the GC, refer to the 7890 GC manual.

NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

Configuring the Driver

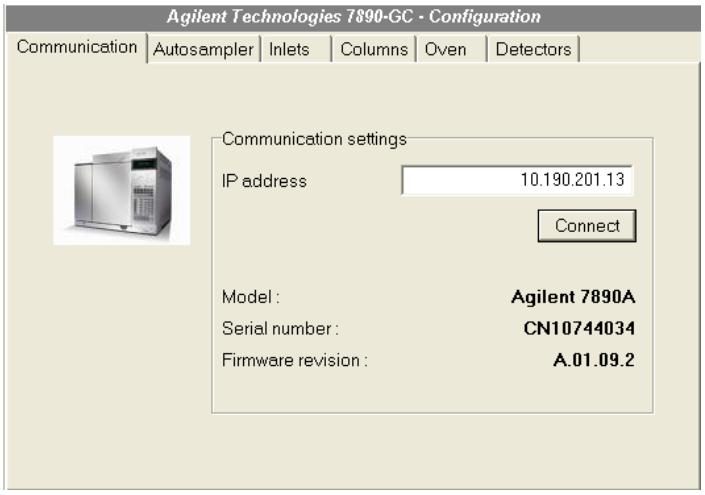
The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

Configuring the Agilent 7890 Gas Chromatograph

Click on the

button corresponding to the Agilent 7890 Gas Chromatograph driver and the configuration screen appears.

Communication Window



Communication settings Parameter Group

IP address:

Type the IP address of the instrument. Once the IP has been correctly typed, press the Connect button to activate the communication with the GC.

Model:

In this field, the model of the 7890 GC is automatically updated when the communication is established.

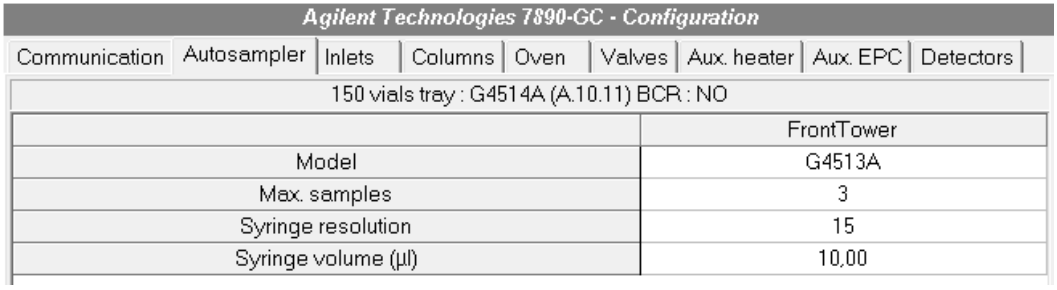
Serial number:

In this field, the serial number of the 7890 GC is automatically updated when the communication is established.

Firmware revision:

In this field, the firmware revision of the 7890 GC is automatically updated when the communication is established.

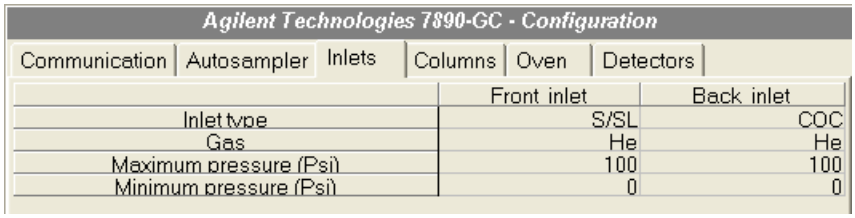
Autosampler Window



The autosampler(s) present on the GC is (are) automatically detected and their parameters are uploaded as follows:

- The sampler model
- The tray model if a tray is configured
- The maximum sample number, depending on the sampler turret model.

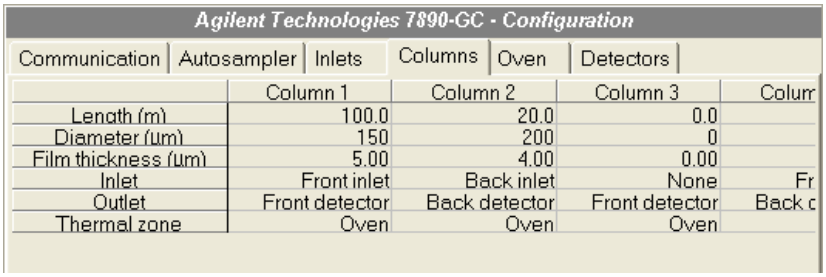
Inlets Window



The inlets present in the GC are automatically detected and their parameters are uploaded. For an S/SL inlet, the gas, the Minimum and the Maximum pressure are uploaded from the GC. For a COC inlet, the gas, the Minimum and the Maximum pressure are uploaded from the GC.

For a MMI inlet, the gas, the Minimum and the Maximum pressure, and the presence of the Cryo and its type are uploaded from the GC.

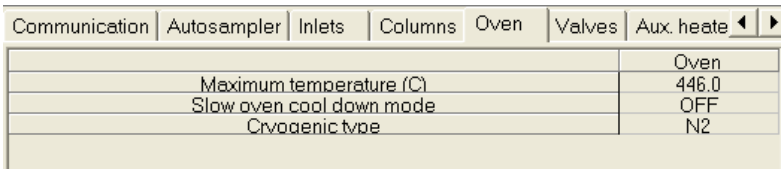
Columns Window



The columns defined on the GC are automatically detected and their parameters are uploaded.

For each column, the length (in meters), the diameter (in micrometers), the film thickness (in micrometers), the associated inlet, the outlet and the thermal zone are uploaded from the GC.

Oven Window

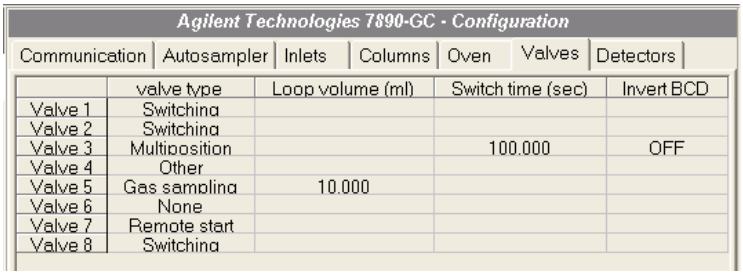


The maximum oven temperature is automatically displayed.

The slow oven cool down mode setting (ON or OFF) is displayed as well. Cryogenic Type is displayed if cryo is installed, with the selected gas.

All these fields are read-only and can only be edited from the GC front panel.

Valves Options Window

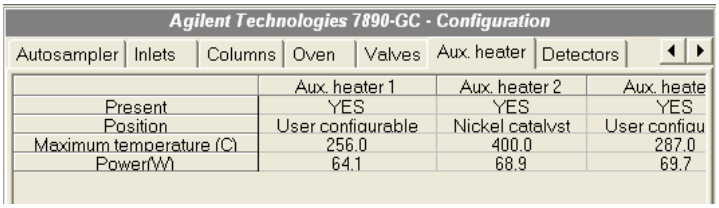


The user can configure up to 8 valves.

Select the Valve Type. Six choices are available: None, Multiposition, Gas sampling, Remote Start, Switching and Other.

- Multiposition: Generally used as a gas stream selection valve, to select one of several gas streams.
- Gas sampling: A run is automatically started when the valve switches from load position to inject position.
- Other: Could be anything.
- Remote Start: to send a start to the GC.
- Switching: Generally used to select one of two columns for analysis.

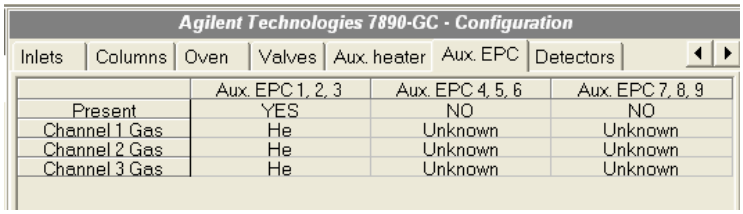
Auxiliary Options Window



The auxiliary thermal controller provides two channels of temperature control. Configure the Auxiliary on the GC.

According to the Aux heater selected on the GC, the maximum temperature can be defined by the user or not. The maximum temperature and the power (calculated by the GC) are listed in the configuration screen, by auxiliary heater.

Auxiliary EPC Options Window



The Auxiliary Pressure Controller (Aux EPC) option. It has three independent forward-pressure regulated channels. Each channel is assigned a number from 1 to 9 (there can be up to 3 Aux EPCs, containing each 3 channels), depending on where the module is installed.

Pressure Control Module Options Window

Communication | Autosampler | Inlets | PCM | Columns | Oven | Valves

	PCM A	PCM B	PCM C
Present	NO	NO	YES
Heater	NO	NO	NO
Channel1 Gas	Unknown	Unknown	N2
Channel2 Gas	Unknown	Unknown	H2
Channel2 Mode	Unknown mode	Unknown mode	Forward pressure

Three Pressure Control Modules (PCM) can be installed (A, B and C). For each one configure on the GC whether a heater is available or not, the gas for channel 1 (PCM on GC) and channel 2 (Aux PCM on GC), for channel2 configure whether it is in forward pressure or Back pressure mode.

Detectors Window

Agilent Technologies 7890-GC - Configuration

Communication | Autosampler | Inlets | PCM | Columns | Oven | Valves | Aux. heater | Aux. EPC | Detectors

	Front detector	Back detector	Aux detector 1 detector	Aux detector 2 detector
Detector type	FID	TCD	TCD	AIB
Fuel gas	H2			
Utility / Reference gas	Air	He	He	
Makeup gas	He	He	He	
Lit offset	2.0			
Auto adjust				
Dry bead				
Blos bead				
Max. bead voltage (V)				

The detectors present in the GC are automatically detected and their parameters are uploaded. For a FID, the 3 gas types (Fuel, Utility and Makeup) and the Lit Offset are uploaded from the GC. For a TCD, the 2 gas types (Utility/reference gas and Makeup) are uploaded from the GC.

For a NPD, the 3 gas types (Fuel, Utility and Makeup), Auto Adjust Bead, Dry bead, Blos Bead, Max Bead Voltage are uploaded from the GC.

For a FPD, the 3 gas types (Fuel, Utility and Makeup) and Lit offset are uploaded from the GC. Auxiliary detectors are also listed in this window. 2 Aux detectors can be configured: TCD and AIB.

Auxiliary detectors are also listed in this window. 2 Aux detectors can be configured: TCD and AIB.

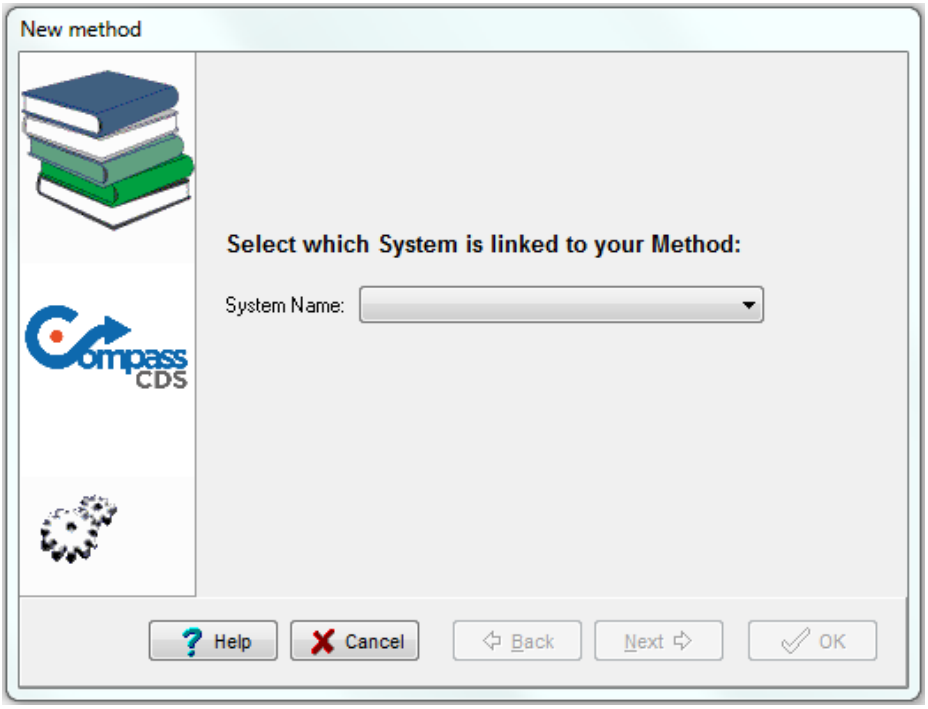
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

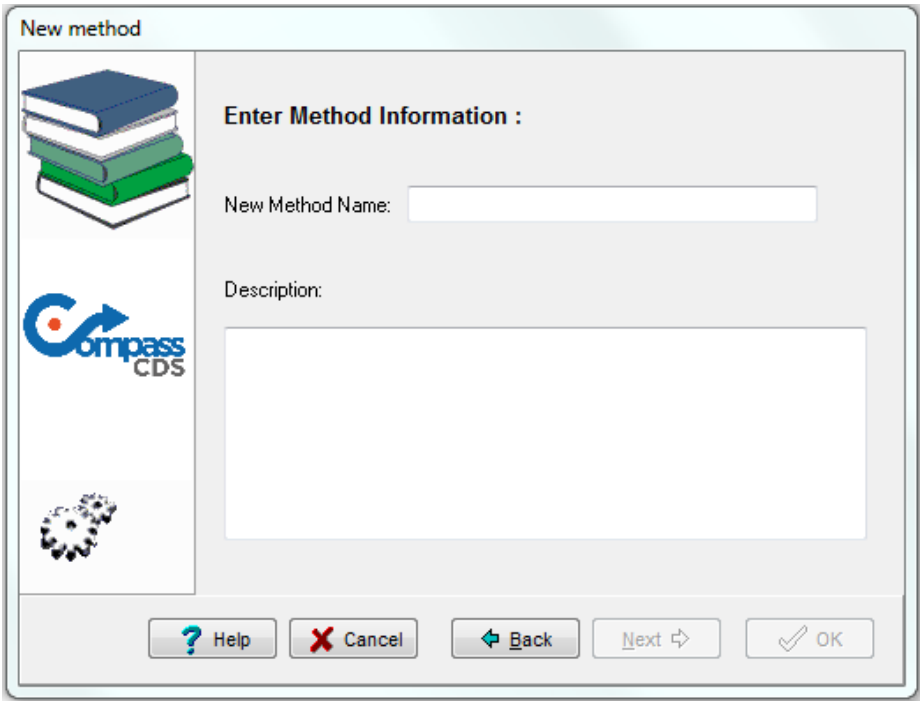
To create a new method, select the ***FILE / NEW METHOD*** option from the CompassCDS Chromatography Data System main menu.

A wizard guide will appear and provide assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

Once this field is completed, click on the Next button to move to the second step of the method creation:



Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

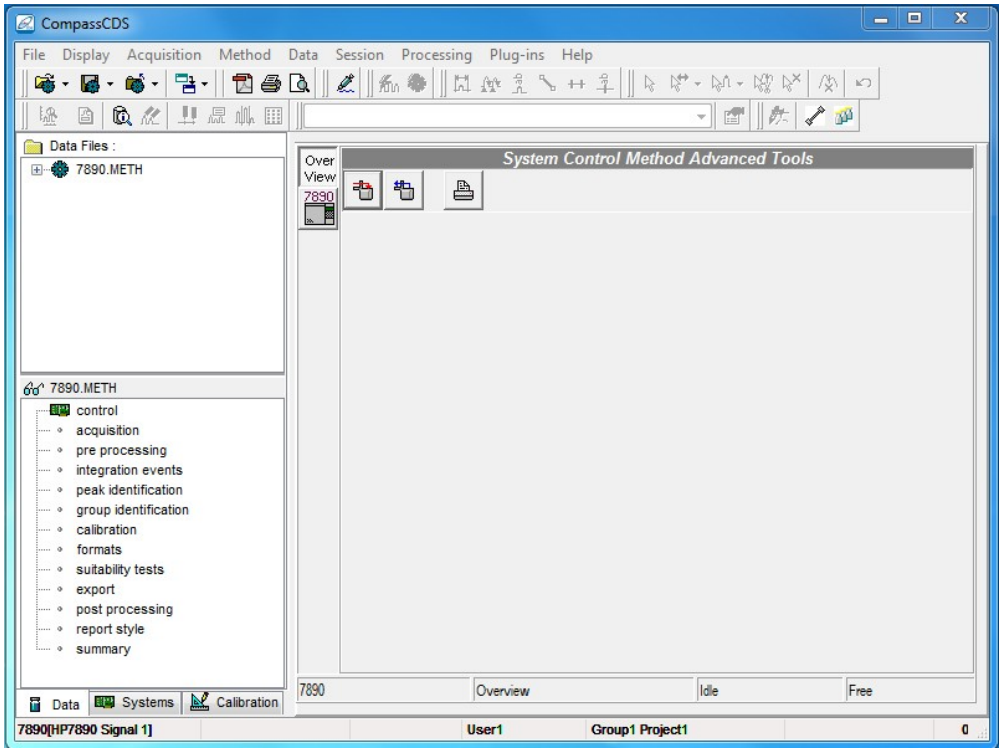
Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

The control section must be defined in order to start an acquisition. In the following part of this guide, only the instrument control section for the Agilent 7890 Gas Chromatograph is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to the CompassCDS Chromatography Data System User Guide.

Control Method Section for the Agilent 7890 Gas Chromatograph

Once the new method is created, select the control section in the lower part of the browser. The following screen appears:



Press the Over View button to display the ***System Control Method Advanced Tools*** window:

to send the current method to the instrument

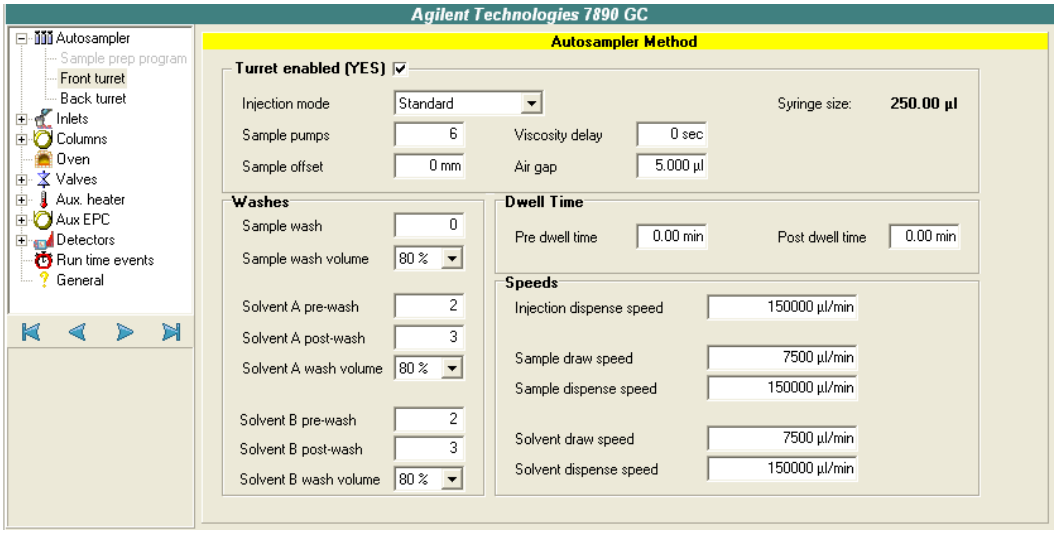
to get the active method from the instrument

to print the current method

Click on the button to display the Agilent 7890 Gas Chromatograph control method section.

It contains 10 sub-sections: *Autosampler, Inlets, Columns, Oven, Valves, Aux .heater, Aux EPC, Detectors, Run time events and General*. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Autosampler Control



Front / Back turret

Depending on the system configuration, select the *Front* or *Back turret* section to set the sampler information of each sub-system.

Injection:

Select the *Enabled* box to activate and consider the *Sampler parameters*.

Select the *Injection mode*: Standard, 2-layer sandwich or 3-layer Sandwich mode in order to use the sandwich injection, Large Volume (LVI).

In the *Sample Pumps* field, enter the number of pumps before the injection (plunger strokes to avoid the formation of bubbles and improve reproducibility).

In the *Sample offset* field, set the variable sampling depth. Set 0 for OFF

In the *Viscosity Delay* field, enter a time (in seconds). During this time, the syringe plunger has a pause between the pumping and the injection stroke. For viscous samples, the pause allows the sample to flow into the vacuum created in the syringe.

Air gap: Field available only if the new Agilent 7693 autosampler is present. Enter in this field, the amount of air separating the sample from the end of the needle.

NOTE: The Air gap values accepted are actually syringe hundredths. For this reason, all values cannot be entered in this field. A message will be displayed if the value is not correct depending on the syringe size.

In the *Injection replicate* field (available for the new Agilent 7693 autosampler when LVI mode is selected), enter the number of injections that will be performed from the same sample, during the same analysis.

In the *Injection* field (available for the new Agilent 7693 autosampler when LVI mode is selected), enter the delay in seconds between two consecutive replicates.

Washes:

In the *Sample wash* field, enter the number of syringe washes with the sample, before injection.

In the *Sample wash volume* field, enter the percentage of the syringe volume that will be filled by the sample during the wash.

In the Solvent A and B Pre-wash fields, enter the number of syringe washes with solvent A and/or B, before injection. In the Solvent A and B Post-wash fields, enter the number of syringe washes with solvent A and/or B, after injection.

In the *Solvent A and B wash volume* fields, enter the percentage of the syringe volume that will be filled by the solvent A or B during the wash.

Dwell Time:

In the *Pre Dwell Time field,* enter the time in minutes the needle stays in the inlet before the injection. In the *Post Dwell Time field*, enter the time in minutes the needle stays in the inlet after the injection.

Speeds:

In the *Injection dispense speed* field, enter the speed of the syringe during injection.

In the *Sample draw speed* field, enter the speed of the syringe when drawing the sample from the vial.

In the S*ample dispense speed* field, enter the speed of the syringe when dispensing the sample in the waste, during the wash step.

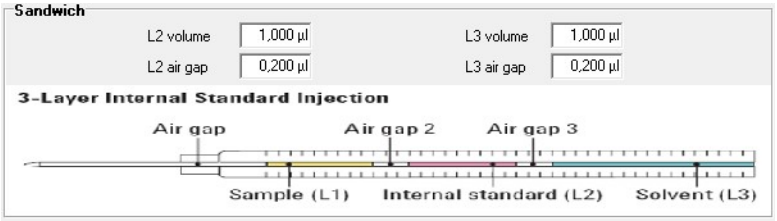
In the *Solvent draw speed* field, enter the speed of the syringe when drawing the solvent from the wash vial.

In the *Solvent dispense speed* field, enter the speed of the syringe when dispensing the solvent in the waste, during the wash step.

NOTE: The speeds values depend on the syringe size. All values will not be taken into account by the GC. For this reason, some values can be entered and the value on the GC can be a little different.

Sandwich:

In 2-layer Sandwich and 3-layer sandwich mode (only available with the new Agilent 7693 autosampler), a new part of the screen is displayed:



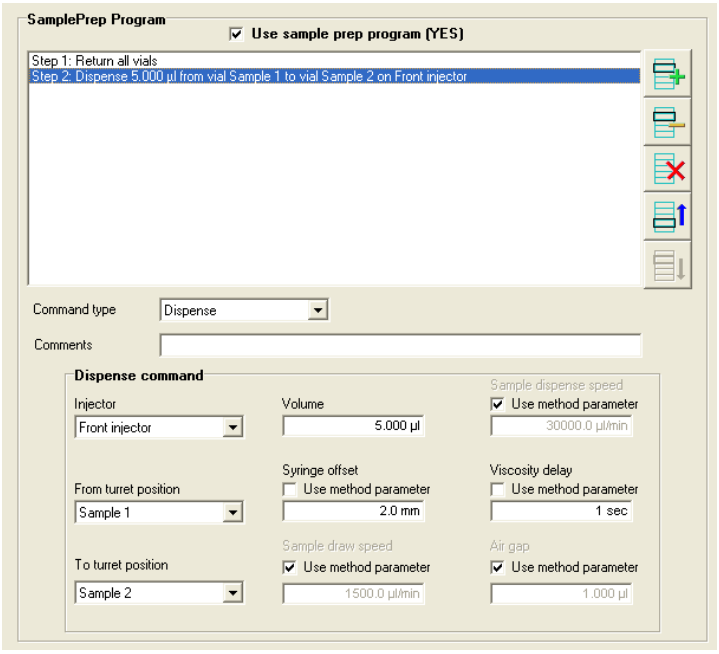
In the *L2 and L3 volume* fields, enter the amount of sample used in layer 2 and/or 3.

In the *L2 Air gap volume* fields, enter the amount of air used between sample layer 1 and sample layer 2. In the *L3 Air gap volume* fields, enter the amount of air used between sample layer 2 and sample layer 3.

NOTE: The Air gap and layer volume values accepted are actually syringe hundredths. For this reason, all values cannot be entered in this field. A message will be displayed if the value is not correct depending on the syringe size.

Sample preparation program

If the 7693 autosampler is installed with the sample tray, you can configure the autosampler to prepare or manipulate samples before running a method. All these sample preparation programs run before any other standard injection and post-injection program.



Several commands are available. For each one a series of parameters have to be set. Some of them can take the values defined in the Front/Back turret part of the method (check Use method parameter) or values entered by the user (uncheck Use method parameter).

Dispense:

The *Dispense* command transfers an amount of fluid from one turret position to another in the same turret. The following dispense parameters are available:

Injector: Select Front or Back injector depending on your configuration.

From turret position: Select the turret position from which you want to acquire the liquid.

To turret position: Select the turret position into which you will dispense the liquid.

Volume: Set the amount of liquid to dispense.

Syringe offset: Set the depth of the syringe needle in the vial.

Draw speed: Set the rate to draw liquid into the syringe.

Dispense speed: Set the rate to dispense liquid into the syringe.

Viscosity delay: Set the amount of seconds the plunger pauses to let the syringe fill with liquid.

Air gap: Set the amount of air that separates the liquid from the end of the needle.

Comments: Enter any information (optional).

Heat:

The *Heat* command controls the heater temperature and the heating time of the vial. The heater remains at the last temperature setting until a new heat step changes it.

The following Heat parameters are available:

Temperature: Define the temperature of the heater. It is possible to maintain the last temperature setting, to turn the heater off or to set a new temperature.

Time: Define the amount of time the vial is heated. It is possible to not wait for the vial to reach a specified temperature before continuing (*No wait* option).

NOTE: This command does not move the vial to and from the heater position. You must use the *Move vial* command before and after *Heat* in your preparation program.

Load:

The *Load* command moves the syringe into a vial and then the plunger to a specified position. It can also be used to fill a syringe and then to partially unload the content into several vials.

The following *Load* parameters are available:

From injector: Select Front or Back injector depending on your configuration.

From turret position: Select the turret position from which you want to acquire the liquid.

Syringe position: Set the syringe position.

Syringe offset: Set the depth of the syringe injection.

Plunger volume: Set the plunger volume to draw a specified volume of liquid into the syringe.

Plunger mode: The plunger volume can be measured by the travel of the plunger stroke (*Relative*) or by the syringe volume reading (*Absolute*).

Plunger speed: Set the rate to draw or dispense liquid.

Delay: Set the time the plunger pauses to let the syringe will with liquid.

Air gap: Set the amount of air that separates the liquid from the end of the needle.

EXAMPLES:

To transfer a liquid, use one *Load* command (relative) to fill the syringe and other *Load* command (absolute) to dispense the desired amounts of liquid into vials or into the inlet.

To dilute a sample, use one *Load* command to draw an amount of solvent and then a *Dispense* command to draw and dispense this mixture of sample and solvent.

To avoid air bubbles, use rather *Load* than *Dispense* as you can, with a Load command expel only a portion of syringe that contains no bubbles.

Mix Sample:

The *Mix Sample* command controls the mixer speed, the mixer direction, the time to mix a vial and the time to wait between mixing cycles.

The following *Mix Sample* parameters are available:

Mode: Set the type of mix cycle, for example bi-directional. *Number of cycles:* Define the number of mix cycles per vial. *Speed*: Define the number of rotations per minute.

Total mixing time: It corresponds to the sum of the mix time and dwell time multiplied by the number of mix cycles.

Mix cycle time: Define the amount of time to mix the vial per mix cycle.

Dwell time: Set the amount of idle time between mix cycles.

NOTE: This command does not move the vial to and from the mixer position. You have to use the *Move vial* command before and after *Mix Sample* in your preparation program.

Move Vial:

The *Move Vial* command instructs the tray to move a vial from one location to another.

From position: Select the position to take the vial.

To position: Select the position to put the vial.

Depending on the configuration of the autosampler, the following move positions may be available:

Tray vial: Select a vial from a fixed position in the rack.

Front or Back turret: Select one of the three transfer positions in the turret.

Heater: Specify the heater if available.

Mixer: Specify the mixer if available.

Pumps:

The *Pumps* command enables the user to perform sample pumps to wet a syringe before use. Pumps can reduce air bubbles in some samples.

The following Pumps parameters are available:

Injector: Select Front or Back injector depending on your configuration.

Turret position: Select the turret position in which you want to perform the pumps.

Number of pumps: Define the number of pumps.

Volume: Set the amount of liquid to draw and dispense. *Syringe offset:* Set the depth of the syringe needle in the vial. *Draw speed:* Set the rate to draw liquid into the syringe.

Dispense speed: Set the rate to dispense liquid into a vial.

Viscosity delay: Set the time the plunger pauses to let the syringe fill with liquid.

Return All:

The *Return All* command returns any vial in the turret, mixer or heater to its original position.

Wait:

The *Wait* command instructs the system to pause for a specified time before continuing with the next command. *Wait* can be used to allow a sample to cool or to hold while a reaction takes place.

Washes:

The *Washes* command draws liquid from one location and expels the entire amount into another location. The following *Washes* parameters are available:

Injector: Select Front or Back injector depending on your configuration.

Solvent wash bottle: Select the turret position from which you want to acquire the wash liquid.

Dispense to: Select the turret position into which you will dispense the liquid.

Number of washes: Select the number of times the syringe is washed.

Volume: Set the wash volume.

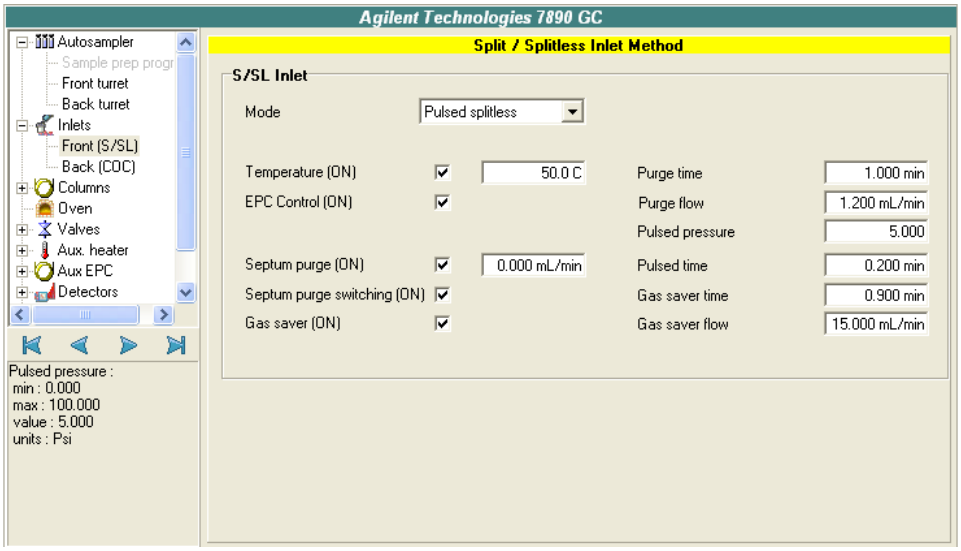
Syringe offset: Set the depth of the syringe injection. *Draw speed*: Set the rate to draw liquid into the syringe. *Dispense speed:* Set the rate to dispense liquid into a vial.

Viscosity delay: Set the time the plunger pauses to let the syringe fill with liquid.

Inlet Control

Depending on the system configuration, select the *Front* or *Back* inlet in the browser

Split/Splitless



Check the *Temperature* box to activate the inlet temperature. Enter the desired *Temperature*.

Check the *EPC Control* to activate it. The pressure has to be set in the Columns section. Inlet pressure is equal to the one of the associated column.

Select the *Injection mode*. The available choices are: *Split*, *Splitless*, *Pulsed split* and *Pulsed splitless*. According to this choice, the following parameters are activated or not.

In the *Septum purge* field, enter the flow in mL/min through the septum purge line. Select the *Septum purge switching* field to activate it.

In the *Total flow* field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined onto the *GC*.

In the *Split ratio* field, enter the ratio between the flow division and column flow. This field is available only if the *Split* and

Pulsed Split inlets are selected.

In the *Purge time field*, enter the time the purge valve is opened. This field is available only if the *Splitless* and *Pulsed Splitless* inlets are selected.

In the *Purge flow* field, enter the flow of the purge vent in mL/min. This field is available only if the *Splitless* and *Pulsed Splitless* inlets are selected.

In the *Pulsed time* field, enter the time the pulsed pressure is maintained in the inlet. This field is available only if the Pulsed

Split and *Pulsed Splitless* inlets are selected.

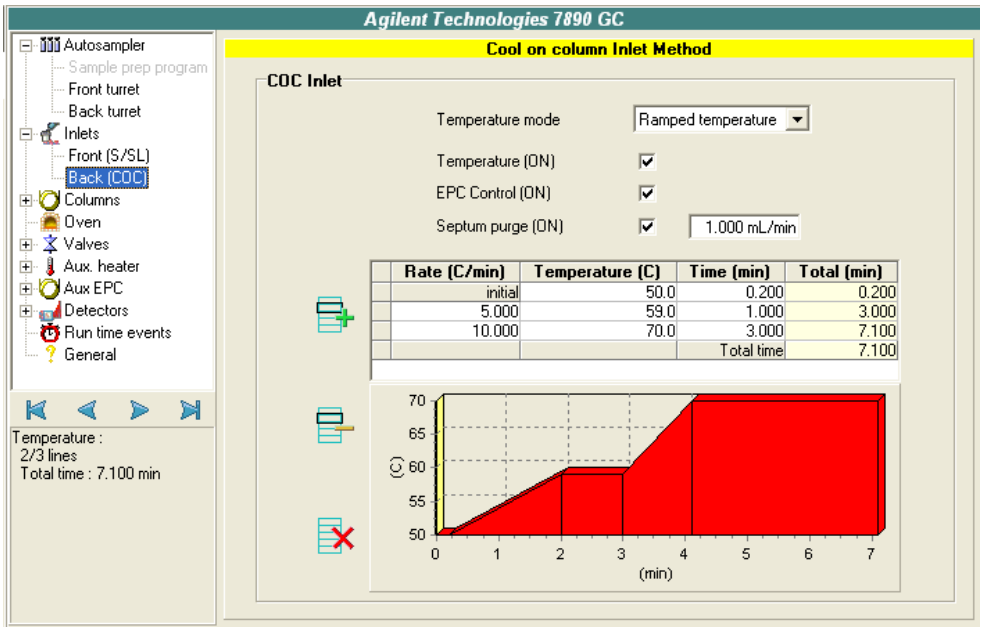
In the *Pulsed pressure* field, enter the inlet pressure when the acquisition starts. This field is available only if the Pulsed *Split* and *Pulsed Splitless* inlets are selected.

Check the *Gas saver* to activate the gas saver. This option is available only if the column parameters have been defined in the *Column* sub-section.

In the Gas s*aver time* field, enter the time the gas saver is activated. This time must be greater than the purge time for splitless injection and greater than the injection time for split injection.

In the Gas s*aver flow* field, enter the gas flow. It must at least equal to column flow, plus 15 mL/min.

Cool On Column

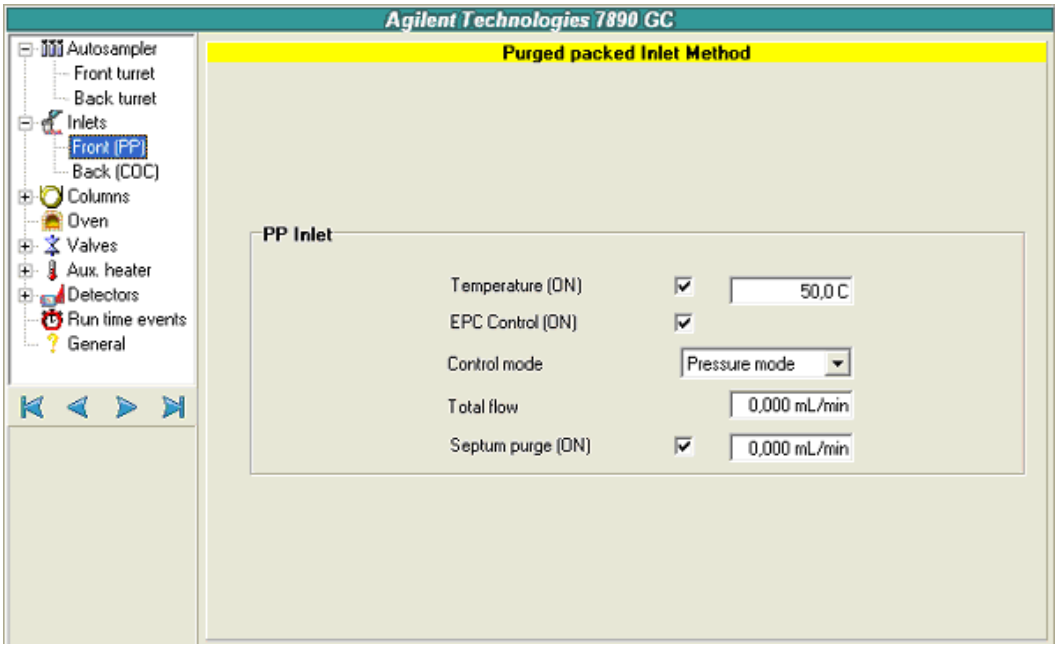


Check the EPC Control box to activate the inlet pressure. The pressure has to be set in the Columns section. Check the Temperature box to turn ON the thermal zone.

- Select the *Track column oven* to make the inlet temperature profile track the oven temperature. The difference between the two temperatures is 3°C.
- Select *Ramped temperature* to set the thermal zone program. In the *Temperature* field, enter the inlet temperature in °C.
- In the *Time* field, enter the time the inlet stays to the *Temperature* in minutes.
- In the *Rate* field, enter the rate in °C/min used to reach the next temperature set point. The total time of the inlet temperature program is displayed in the *Total* field.

The graphic displays the temperature program. Check Septum purge and define the flow in mL/min.

Purged Packed



Check the *Temperature* box to activate the inlet temperature. Enter the inlet temperature in °C.

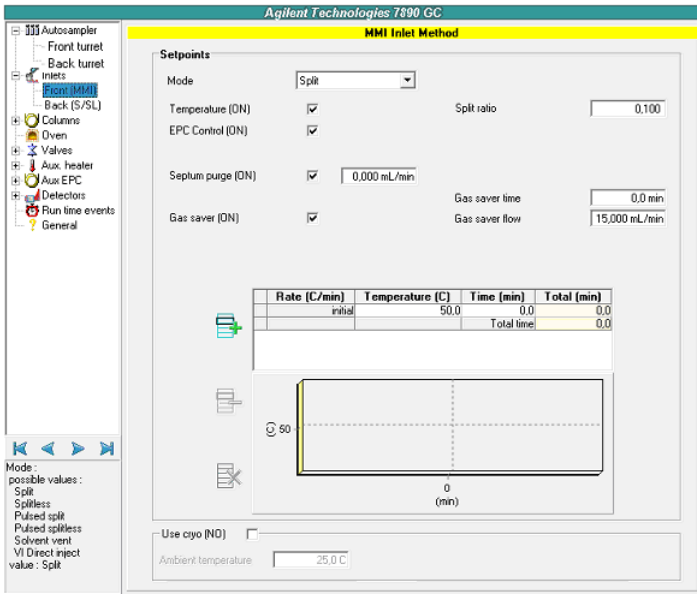
Check the *EPC Control* to activate it. The pressure has to be set in the *Columns* section. Inlet pressure is equal to the one of the associated column.

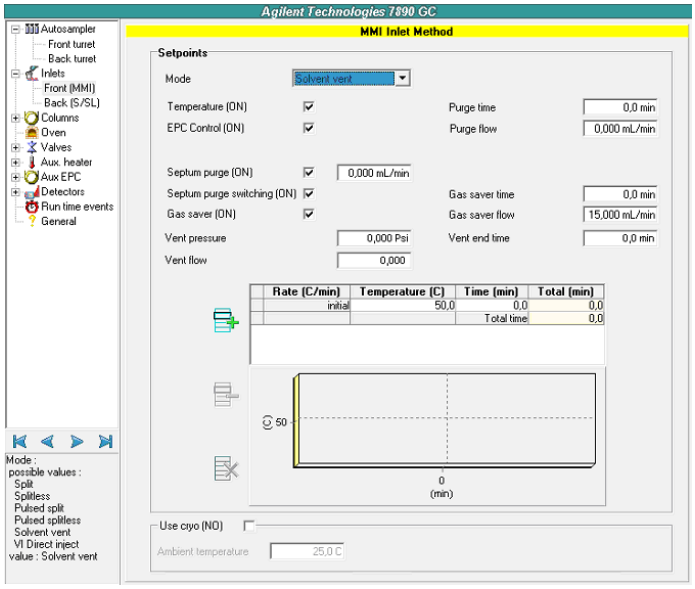
In the *Control mode*, select the desired pneumatic control mode (pressure mode, flow mode).

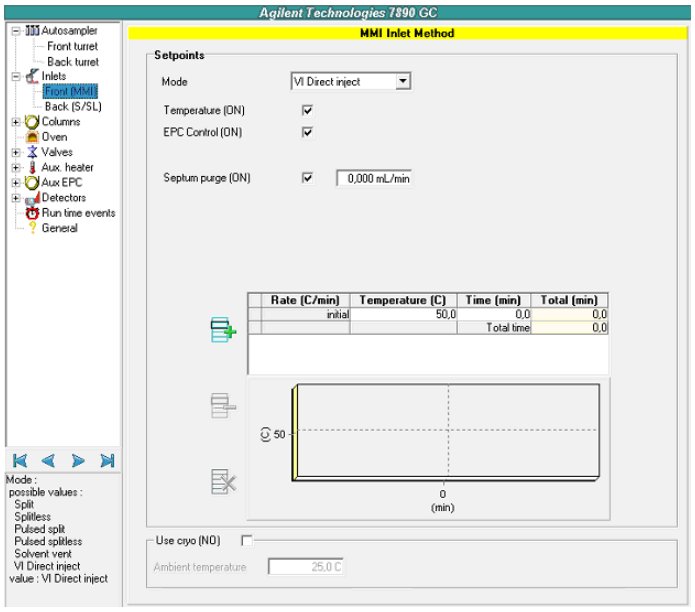
In the *Total flow* field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined onto the *GC*.

In the *Septum purge* field, enter the flow in mL/min through the septum purge line.

Multi Mode Inlet (MMI)







The MMI inlet control screen uses the same one than the Slit/Splitless with a temperature program available and the Cryo available if needed.

Select the *Injection mode*. The available choices are: *Split*, *Splitless*, *Pulsed split*, *Pulsed splitless, Solvent vent and VI Direct inject*. Depending upon this choice, the following parameters are activated or not.

Split, Splitless, Pulsed split, Pulsed splitless

Please refer to the *Split/Splitless* inlet part of this manual.

In the *Temperature* field, enter the inlet temperature in °C.

In the *Time* field, enter the time the inlet stays to the *Temperature* in minutes.

In the *Rate* field, enter the rate in °C/min used to reach the next temperature set-point. The total time of the inlet temperature program is displayed in the *Total* field.

The graphic displays the temperature program.

Check the *Use cryo* box to activate the cyo, and set the ambient temperature.

Solvent vent mode:

Check the *Temperature* box to activate the inlet temperature. Enter the desired *Temperature*.

Check the EPC Control to activate it. The pressure has to be set in the Columns section. Inlet pressure is equals to the one of the associated column.

In the *Septum purge* field, enter the flow in mL/min through the septum purge line. Select the *Septum purge switching* field, to activate it.

In the *Total flow* field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined onto the *GC*.

In the *Purge time field*, enter the time the purge valve is opened. This field is available only if the *Splitless* and *Pulsed Splitless* inlets are selected.

In the *Purge flow* field, enter the flow of the purge vent in mL/min. This field is available only if the *Splitless* and *Pulsed Splitless* inlets are selected.

In the *Total flow* field, enter the sum of the division flow, the column flow and the septum purge flow. This field is available only if the column parameters have not been defined onto the *GC*.

Check the *Gas saver* to activate the gas saver. This option is available only if the column parameters have been defined in the *Column* sub-section.

In the Gas s*aver time* field, enter the time the gas saver is activated. This time must be greater than the purge time for splitless injection and greater than the injection time for split injection.

In the Gas s*aver* f*low* field, enter the gas flow. It must at least equal to column flow, plus 15 mL/min.

In the *Vent pressure* field, enter the inlet pressure during the vent period. By decreasing the inlet pressure while venting, solvent elimination proceeds faster. Also, the pressure reduction decreases the amount of carrier gas and solvent vapor that enters the column during this time. If 0 is chosen, the inlet uses the lowest pressure possible at the given vent flow. Please refer the Instrument manual to know more about this feature in the GC.

In the *Vent flow* field, enter the flow of carrier gas out the split vent during the vent period.

In the *Vent end time* field, enter the time, measured from Start Run, when solvent venting ends. For large volume injections, this time is normally greater than the time for the injection to complete.

In the Temperature field, enter the inlet temperature in °C.

In the Time field, enter the time the inlet stays to the Temperature in minutes.

In the Rate field, enter the rate in °C/min used to reach the next temperature set-point. The total time of the inlet temperature program is displayed in the Total field.

The graphic displays the temperature program.

Check the Use cryo box to activate the cyo, and set the ambient temperature.

VI Direct Inject:

Check the Temperature box to activate the inlet temperature. Enter the inlet temperature in °C.

Check the EPC Control box to activate the inlet pressure. The pressure has to be set in the Columns section. In the Septum purge field, enter the flow in mL/min through the septum purge line.

In the *Temperature* field, enter the inlet temperature in °C.

In the *Time* field, enter the time the inlet stays to the *Temperature* in minutes.

In the *Rate* field, enter the rate in °C/min used to reach the next temperature set-point. The total time of the inlet temperature program is displayed in the *Total* field.

The graphic displays the temperature program.

Check the *Use cryo* box to activate the cryo, and set the ambient temperature.

Column Control

Depending on the system configuration, select the *column number* in the browser.

NOTE: If several columns are associated to the same inlet, only the first one can be configured. If selecting the other ones in the browser, the following sentence is displayed: *Warning: Another column is connected to the same Inlet. Column is ignored.*

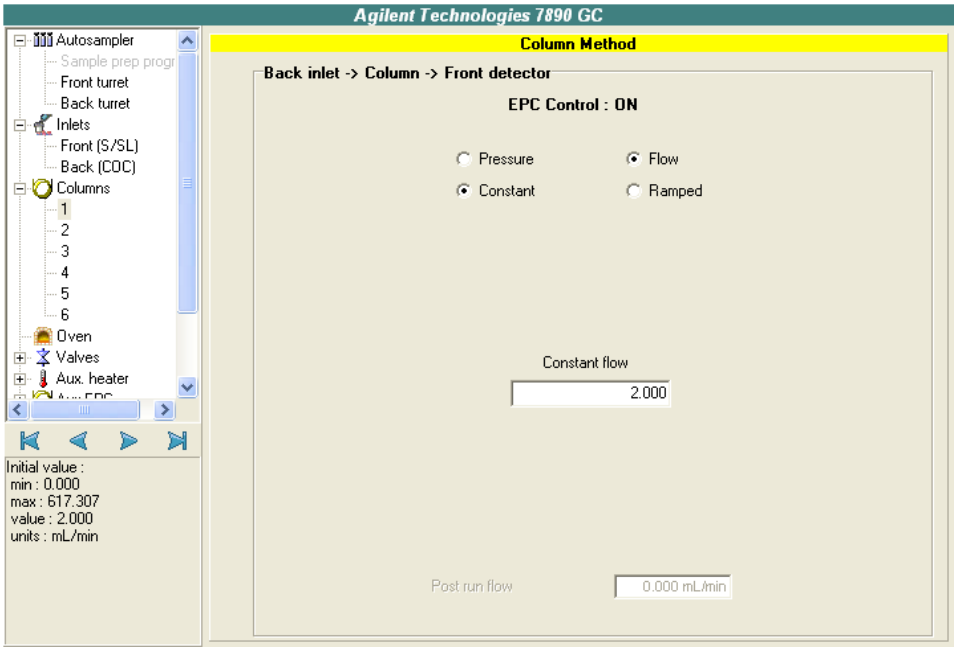
If a column is not associated to an inlet in the GC configuration, the corresponding column screen is not available.

If *EPC Control* option is checked in the Inlet session *EPC Control: ON* is displayed. If *EPC Control* option is not checked in the Inlet session *EPC Control: OFF* is displayed.

The user can choose to work either in Pressure or Flow control. In both cases he can select either constant or ramped flow.

NOTE: If column parameters are not defined in the GC (Length, Diameter, Film thickness), the Flow option is not available

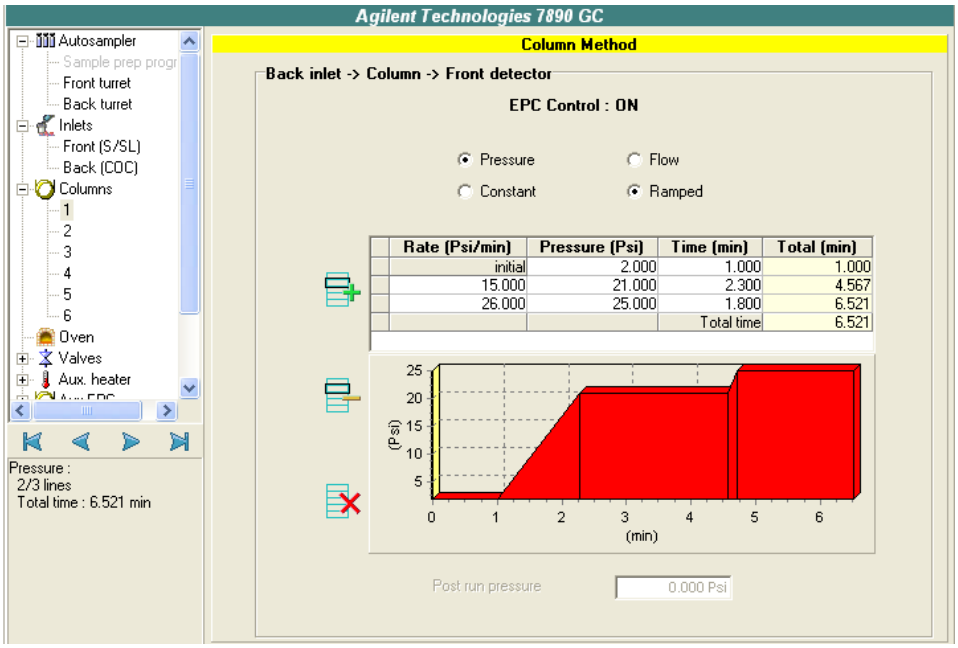
---



Select *Pressure* and *Constant* to maintain a constant pressure in the column. Then enter the corresponding pressure or flow in the *Pressure* or *Flow* fields.

Select *Flow* and *Constant* to maintain a constant flow in the column. Then enter the corresponding flow or pressure in the *Flow* or *Pressure* fields.

In case of *Ramped Pressure* or *Ramped Flow*, the user has to define the program in the table. The table is limited to four lines.



Select Pressure and Ramped to set a pressure program.

In the table program the rate, the plateau pressure, and the duration of the column plateau pressure. The graphic displays the pressure program.

The total time of the program is displayed in the Total field.

Define the pressure at the column ends in the Post run pressure field.

Select Flow and Ramped to set a flow program in the column.

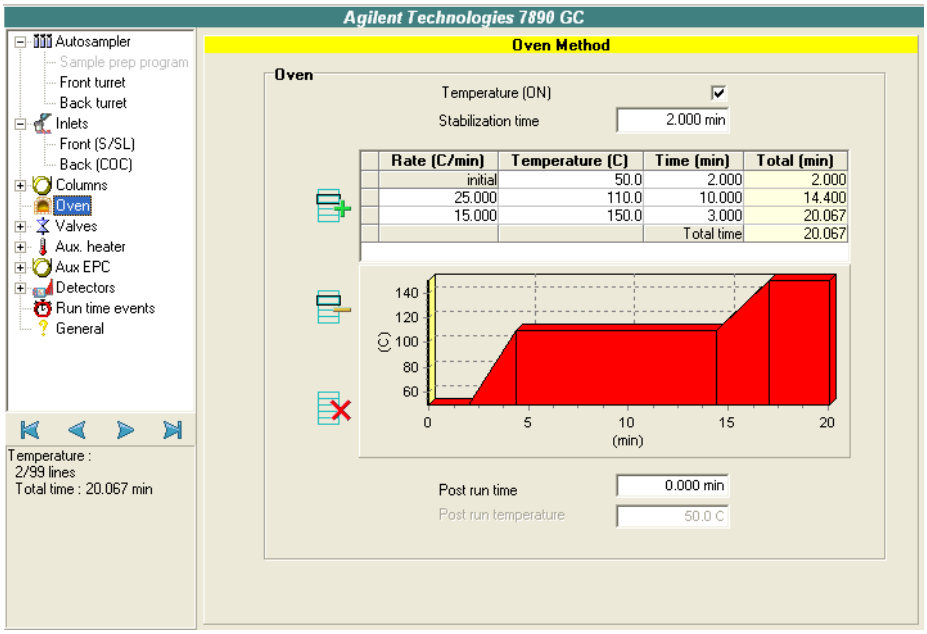
In the table program the rate, the plateau flow, and the duration of the column plateau flow. The graphic displays flow program.

The total time of the program is displayed in the Total field.

Define the flow during the post run period in the Post run flow field.

NOTE: Setting the Flow ramp, the limit of the column flow is [-150.000 .. 150.000]. The flow is not computed depending on the column size. It is the user's responsibility to set up a column flow that is correct for the column size.

Oven Control



Check the *Temperature* box to turn the oven ON and control its temperature. If the box is unchecked, all the following oven parameters will be grayed.

In the *Stabilization Time* field, enter the time before the GC becomes ready in minutes.

In the table, program the rates, the plateau temperatures, and the duration of the oven plateau temperature. The graphic below the table displays the oven temperature program.

The total time of the oven program is displayed in the *Total Time* field.

If a Cryogenic cooling is installed, the following parameters are displayed:

Use cryo: select this option to use the Cryogenic cooling.

Ambient temperature: This setpoint defines the temperature at which cryogenic cooling is enabled.

Fault detection: If the temperature has not been reached after 16 min of continuous Cryogenic operation, the oven is shutting down.

Timeout detection: If no run is started during the *Timeout* (min), the Cryo is shutting down to spare gas.

Timeout: timeout is used by the 'Timeout detection' option.

Quickcool: this option is used to cool the oven faster after a run than it would.

NOTE: If cryogenic module is used to cool the oven, the minimum limit of temperature authorized in the temperature table is decreased. The lower limit depends on the gas used for cryo. For example the lower limit if using N_2 is -80°C.

Post run time: set a time to have a post run period at the end of the normal run. If it is set to zero, no post run is done.

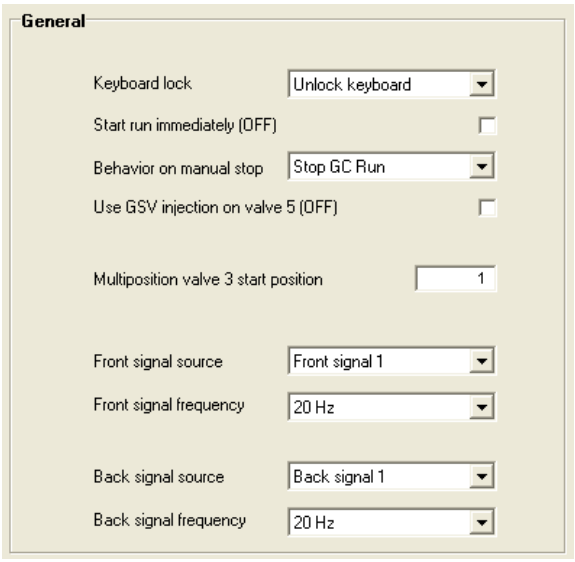
Post-run temperature: defines the oven temperature during the post run period.

Valves Control

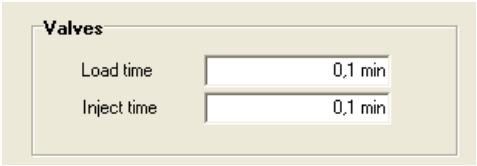
The instrument can have up to eight valves configured. The different fields depend on system configuration. Four types of valves exist: G*as sampling, Multiposition*, *Remote start* and *Switching valves*.

Multiposition Valve Parameters

No parameter has to be set in the Valves section of the control method. The valve start position has to be set in the General section.



Gas Sampling Valve Parameters



In the *Load time* field, enter the time the valve stays in load position.

In the *Inject time* field, enter the time the valve stays in inject position. As soon as the inject time begins, the acquisition starts.

Remote start Valve Parameters

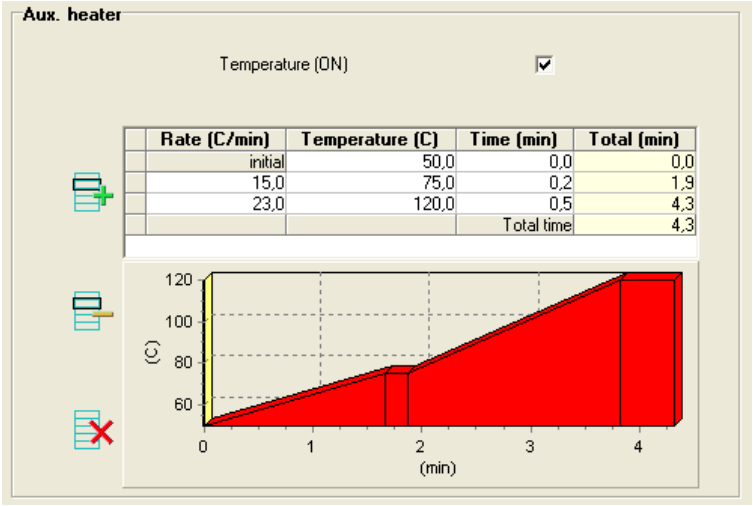
No parameter has to be set.

Switching Valve Parameters

Check the Valve On checkbox to activate the valve. It allows the switching of the valve from one position to another. An event can be added in the event table to switch the valve during a run.

Auxiliary heaters Control

Three auxiliary heaters can be configured, for each one the following screen is displayed:



Check the *On* box to enable temperature programming.

In the *Initial Temperature* field, enter the initial temperature in °C.

In the *Initial Time* field, enter the time the heater block stays to the *Initial Temperature* (first plateau) in minutes.

In the table program the rates, the plateau temperatures, and the duration of the heater block plateau temperature. The graphic displays the temperature program.

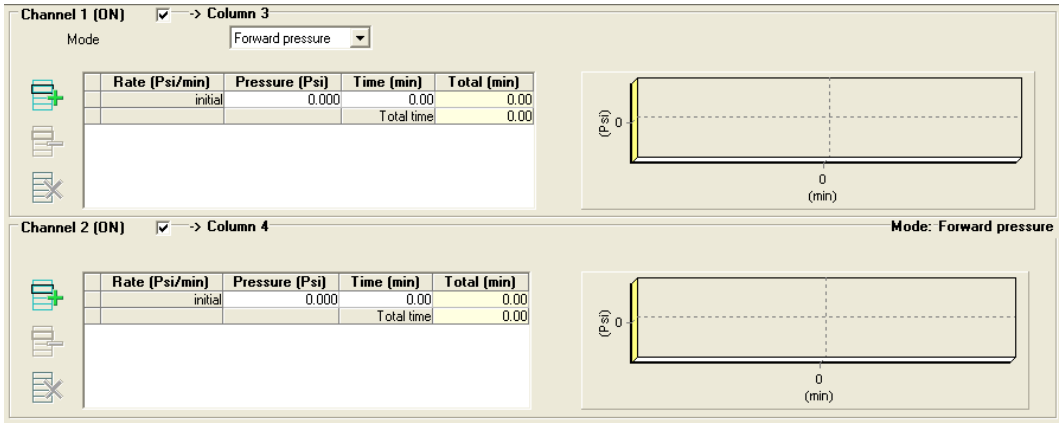
The total time of the heater block program is displayed in the *Total Time* field.

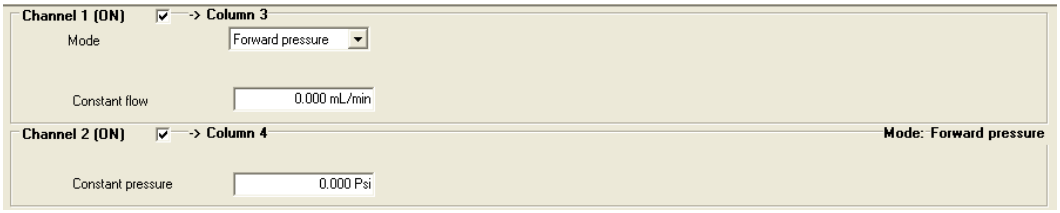
Pressure Control Module

Three PCM modules can be defined (A, B and C). Each PCM owns two independent control channels.

Channel 1 is a simple forward pressure regulator channel that maintains constant the flow or the pressure thanks to a flow sensor or a pressure sensor.

Channel 2 may be used in two modes: forward pressure regulator or back pressure regulator. The configuration has to be defined on the GC, and cannot be modified within the method.





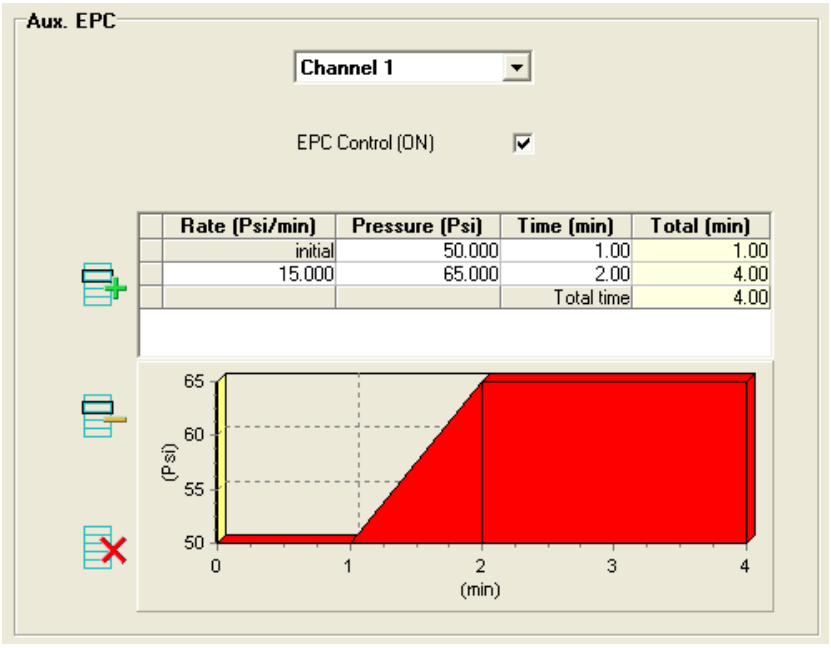
In channel 1 section, select Forward pressure or Flow pressure either you want to fix the pressure or the flow.

In channel 2, only pressure program or constant pressure can be defined. The mode (forward or back pressure) is indicated but cannot be modified from the method.

In the case a column is linked to a PCM in INPUT, the corresponding column screen is linked to the PCM screen, that means that pressure or flow values are identical in both PCM and column screens.

Auxiliary Pressure Control

Three channels are available by Aux. EPC, for each channel the following screen is displayed:



Select the channel to configure into the scrolling list. Then check the ON box to enable EPC Control. In the Initial Pressure field, enter the initial pressure in Psi.

In the Initial Time field, enter the time the EPC block stays to the Initial Pressure (first plateau) in minutes. In the table program the rates, the pressures, and the duration of the EPC block plateau pressure.

The graphic displays the pressure program.

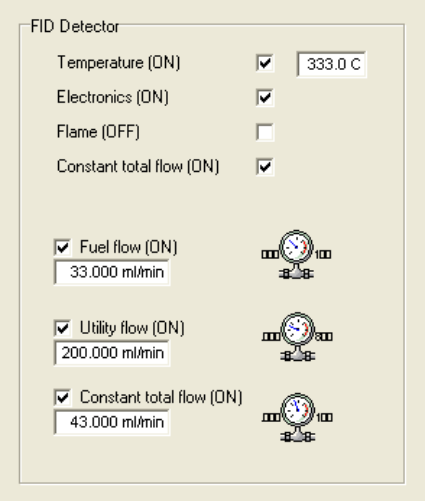
The total time of the EPC block program is displayed in the Total Time field.

Detector Control

Depending on the system configuration, select the Front or Back button, to set the information for each detector. The different fields depend on system configuration.

Auxiliary detectors have to be configured in the detectors part of the method. Aux Det 1 can only be a TCD (Thermal Conductivity detector). Aux Det2 can only be an AIB (Analog Input Board).

FID (Flame Ionization Detector)



Check the *Temperature* box if the temperature control will be used. If the temperature control is ON, define the value in the corresponding field.

Check the *Electronics* box if the electronics control will be used.

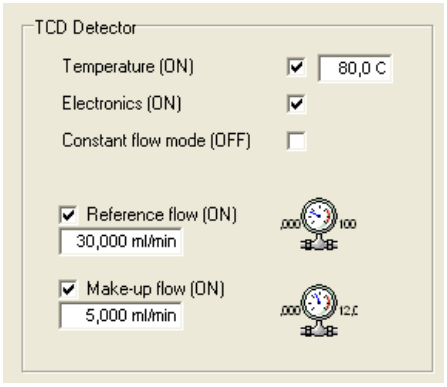
Check the *Flame* box if the method requires to switch the detector flame on.

Check the *Constant total flow* box if the method requires that the total flow (i.e., Make-Up Flow + Column Flow) is constant. Check the *Fuel Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Utility Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Make-up (or Constant total) Flow* box, to control this flow and define the constant value in the corresponding field.

TCD (Thermal Conductivity Detector)



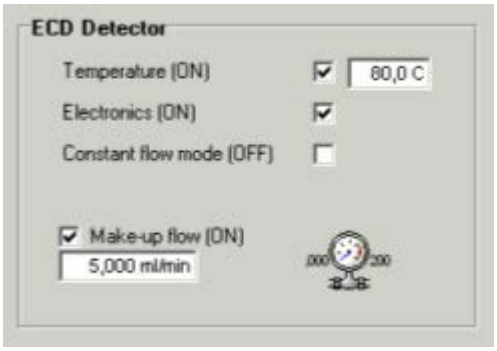
Check the *Temperature* box if the temperature control will be used. If the temperature control is ON, define the value in the corresponding field.

Check the *Electronics* box if the electronics control will be used.

Check the *Constant total flow* box if the method requires that the total flow (i.e., MakeUp Flow + Column Flow) is constant. Check the *Reference Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Make-up (or Constant total) Flow* box, to control this flow and define the constant value in the corresponding field.

ECD (Electron Capture Detector)

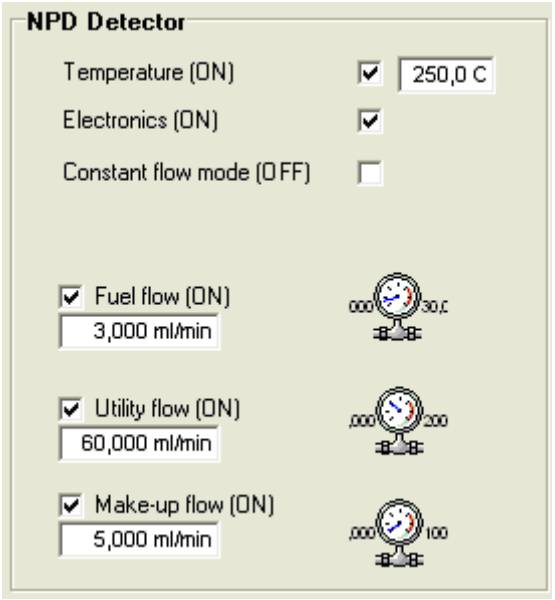


Check the *Temperature* check box to turn the heater ON and define the expected temperature. Check the *Electronics* check box to turn the electrometer ON

Check the *Constant flow* ON check box to force the *Make-Up Flow* + *Column Flow* to be constant. The *Constant total flow* field appears. Define the expected Total flow in mL/min.

Check the *Make-up flow* check box and define a flow if you want to use a make-up gas.

NPD (Nitrogen Phosphorous Detector)



Check the *Temperature* box if the temperature control will be used. If the temperature control is ON, define the value in the corresponding field.

Check the *Electronics* box if the electronics control will be used.

Check the *Constant total flow* box if the method requires that the total flow (i.e., Make-Up Flow + Column Flow) is constant. Check the *Fuel Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Utility Flow* box, to control this flow and define the constant value in the corresponding field.

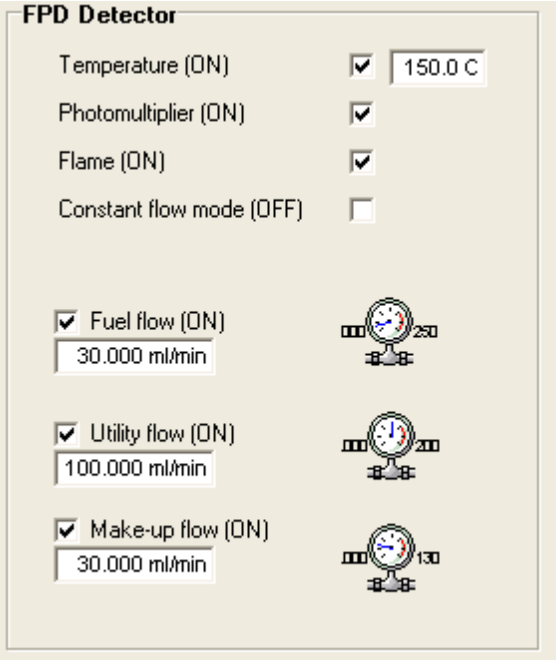
Check the *Make-up (or Constant total) Flow* box, to control this flow and define the constant value in the corresponding field.

NOTE: The *Bead Voltage value used* to heat the bead is not controlled by the driver, the value has to be set on the GC.

AIB (Analog Input Board)

AIB detector is used to recover an analog signal from a non-Agilent detector or other source. The AIB convert the analog signal into a digital signal. No dedicated parameter has to be set in the method, except the acquisition frequency (general section).

FPD (Flame Photometric Detector)



Check the *Temperature* box if the temperature control will be used. If the temperature control is ON, define the value in the corresponding field.

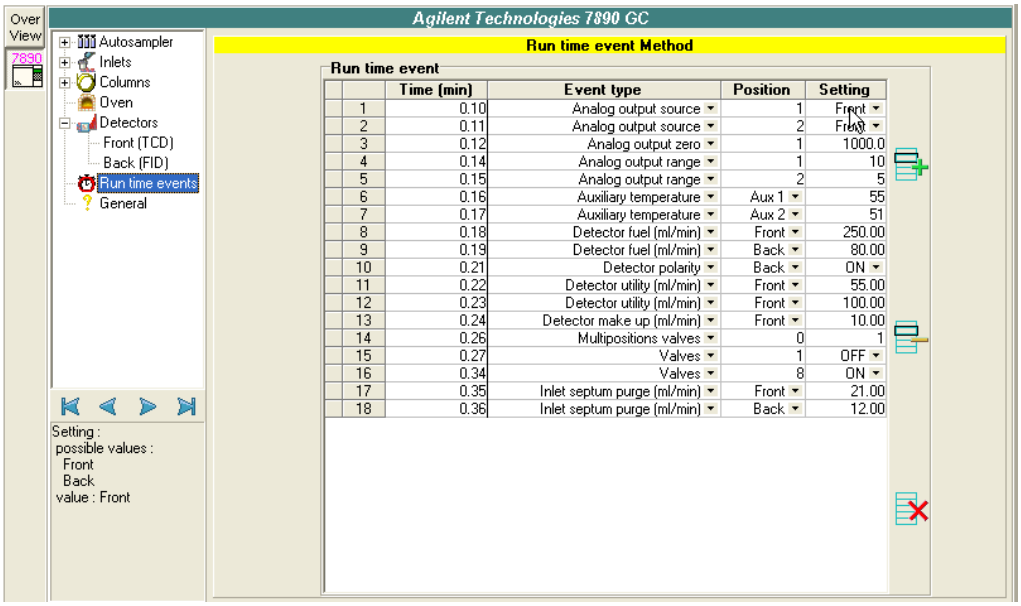
Check the Photomultiplier (*PMT)* box if the electronics control will be used. Check the *Flame* box if the method requires to switch the detector flame on.

Check the *Constant total flow* box if the method requires that the total flow (i.e,. Make-Up Flow + Column Flow) is constant. Check the *Fuel Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Utility Flow* box, to control this flow and define the constant value in the corresponding field.

Check the *Make-up (or Constant total) Flow* box, to control this flow and define the constant value in the corresponding field.

Events Control


Agilent Technologies 7890 GC
Over View
Autosampler
Inlets
Columns
Oven
Detectors
Front (TCD)
Back (FID)
Run time events
General
Setting :
possible values :
Front
Back
value : Front
Run time event Method
Run time event
Time (min) | Event type | Position | Setting
1 | 0.10 | Analog output source | 1 | Front
2 | 0.11 | Analog output source | 2 | Front
3 | 0.12 | Analog output zero | 1 | 1000.0
4 | 0.14 | Analog output range | 1 | 10
5 | 0.15 | Analog output range | 2 | 5
6 | 0.16 | Auxiliary temperature | Aux 1 | 55
7 | 0.17 | Auxiliary temperature | Aux 2 | 51
8 | 0.18 | Detector fuel (ml/min) | Front | 250.00
9 | 0.19 | Detector fuel (ml/min) | Back | 80.00
10 | 0.21 | Detector polarity | Back | ON
11 | 0.22 | Detector utility (ml/min) | Front | 55.00
12 | 0.23 | Detector utility (ml/min) | Front | 100.00
13 | 0.24 | Detector make up (ml/min) | Front | 10.00
14 | 0.26 | Multipositions valves | 0 | 1
15 | 0.27 | Valves | 1 | OFF
16 | 0.34 | Valves | 8 | ON
17 | 0.35 | Inlet septum purge (ml/min) | Front | 21.00
18 | 0.36 | Inlet septum purge (ml/min) | Back | 12.00

In this table program events like valve switching, detector gas flow, TCD polarity change, etc.

NOTE: If the valve rotation is programmed with the event table, it would be better to program the initial position at the end of the analysis.

Use the following buttons to edit the table:

to add a line to the table

to delete a line in the table

to clear the entire table

In the Time column, enter the time when the action has to be done.

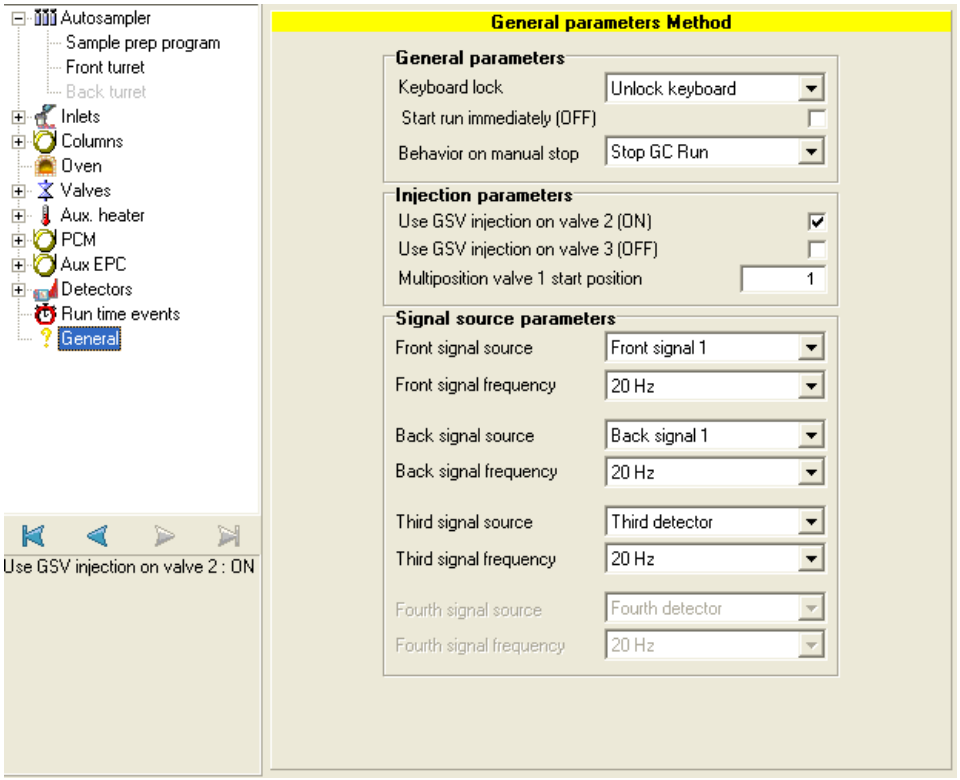
In the Action column, select the action to do. The available choices are:

Analog output source
Analog output auto-zero
Analog output range
Auxiliary temperature
Detector polarity
Detector fuel (=gas 1) (mL/min)
Detector utility (=gas 2) (mL/min)
Detector make up (=gas 3) (mL/min)
Multiposition valve
Valves
Inlet septum purge (mL/min)

In the Position column, select the expected position: Front/Back, ON/OFF, valve #, Aux # …

In the Parameter column, define the expected value / setting.

General Control



Select the lock keyboard mode. 3 choices are available:

Unlock keyboard: All the buttons on the GC front panel are available (including [START], [STOP] …) and all parameters can be edited (temperature set points, flows …).

Lock entire keyboard: no parameter can be edited (temperature set points, flows …) and no action can be done: [START], [STOP] buttons are not active.

Lock keyboard, Start allowed: no parameter can be edited (temperature set points, flows …) and the only action that can be performed is the start of a run: the [START] button is the only active one.

Check ***Start Run Immediately*** to launch an analysis as soon as the GC is ready, without manually starting the GC (with GSV gas sampling valve).

In the ***Behavior on manual stop*** section, select in the scrolling list the expected GC behavior after a manual stop of the run (from CompassCDS acquisition view). If “Let GC continue run” is selected, the GC will complete its oven time program, if “Stop GC run” is selected, the GC will immediately stop its oven program and the system is immediately turned to “Idle”.

Activate or not the ***Use GSV injection on valve X*** section, to inject the sample from a Gas Sampling valve instead of a manual injector or an autosampler.

In the ***Multiposition valve X start*** section, define the position in which the Multiposition valve must be turn on before the injection.

In the ***signal source*** fields, select the acquired signal on the corresponding channel from the list.

Select the acquisition frequency in the *signal frequency* field. The available choices are: *5, 10, 20*, *50*, *100, 200* or *500 Hz*.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

IMPORTANT NOTE: The 7890 is by default in “Auto Prep Run” mode. This prevents any download of CompassCDS methods, thus, any acquisition. Before starting an acquisition, it is then required to remove this setting. To do so, on the GC, press the Config button and edit the Instrument menu. Change the setting of the Auto Prep Run parameter to Off.

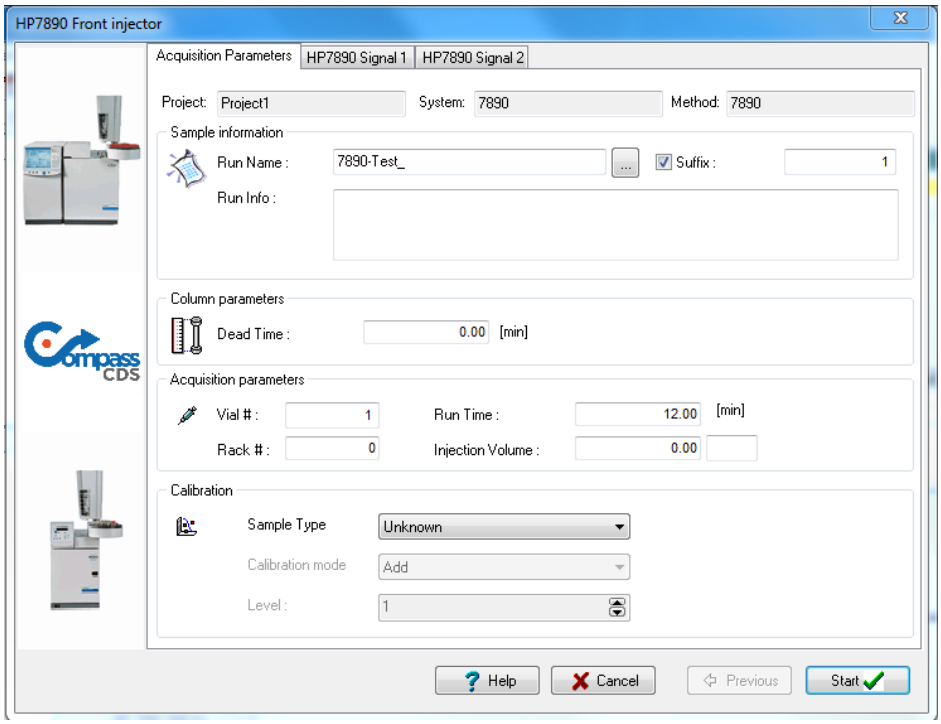
Quick Start (Single Acquisition)

Press the button.

In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

Press the OK button.

The following screen is displayed:



In the *Acquisition parameters* tab, required fields like the *Run Name*, the *Run ID* and the *Acquisition length* must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the *Injection Volume*, the *Vial* position and the *Rack* number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the *Channel X* tab.

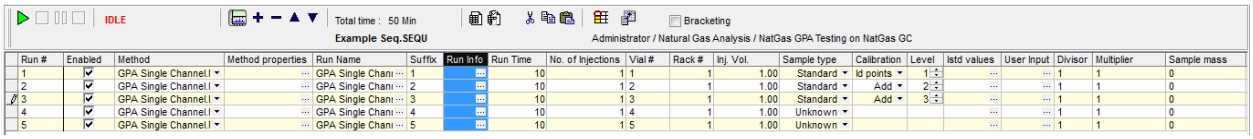
NOTE: The volume that will be injected depends on the Autosampler model (if one is controlled by CompassCDS). See Appendix for details.

Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data System User Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS Chromatography Data System User Guide).



Run #	Enabled	Method	Method properties	Run Name	Suffix	Run Info	Run Time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type	Calibration	Level	Istd values	User Input	Divisor	Multiplier	Sample mass
1	☑	GPA Single Channel.I		GPA Single Chani	1		10	1	1	1	1.00	Standard	Id points	1			1	1	0
2	☑	GPA Single Channel.I		GPA Single Chani	2		10	1	2	1	1.00	Standard	Add	2			1	1	0
3	☑	GPA Single Channel.I		GPA Single Chani	3		10	1	3	1	1.00	Standard	Add	3			1	1	0
4	☑	GPA Single Channel.I		GPA Single Chani	4		10	1	4	1	1.00	Unknown					1	1	0
5	☑	GPA Single Channel.I		GPA Single Chani	5		10	1	5	1	1.00	Unknown					1	1	0

The *Method Name*, the *Run Name*, the *Run ID,* and the *Acquisition length* must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS User Guide.

NOTE: The volume that will be injected depends on the Autosampler model (if one is controlled by CompassCDS). See Appendix for details.

Running Acquisition Status

Viewing a Running Acquisition

To view a running acquisition, click on the *Systems* tab then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

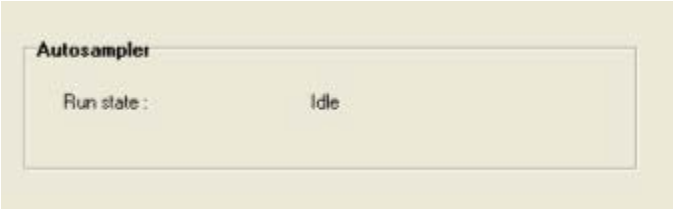
Status of the Agilent 7890 Gas Chromatograph

Click on the

button corresponding to the Agilent 7890 Gas Chromatograph driver and the Agilent Technologies 7890 Gas Chromatograph status screen will appear.

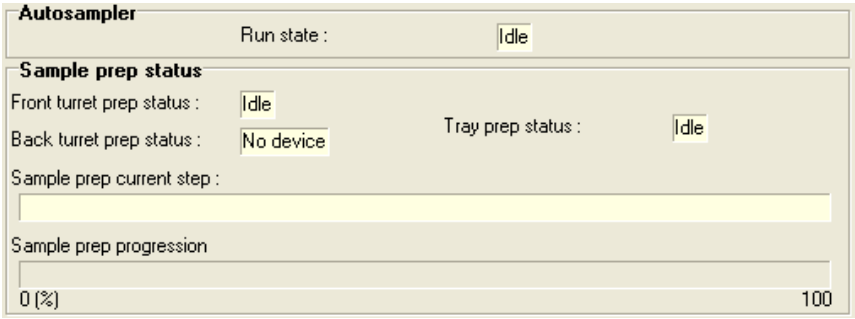
Click on the correct node in the tree-view to display the corresponding screen.

Autosampler:



The actual autosampler state is displayed.

If a 7693 autosampler is installed (prep sample option), the status displays the following information:

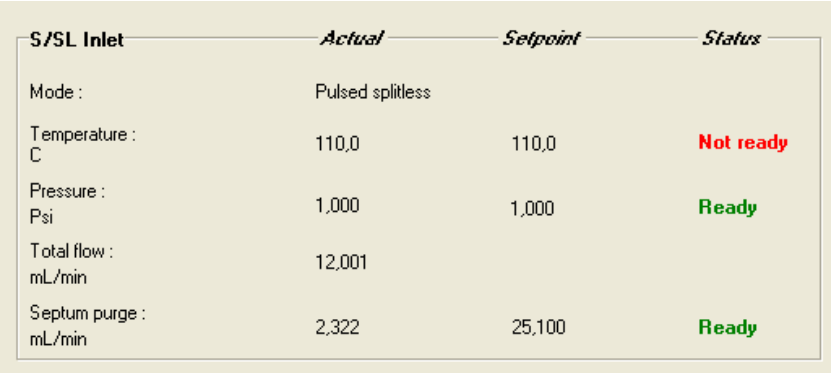


The Sample prep current step displays the action realized by the autosampler, corresponding to the sample prep program defined in the method.

The sample prep progression field displays the evolution of the sample preparation (number of steps done / total number of step).

Inlets:

Split / Splitless



The actual and setpoint values of the Inlet Temperature are displayed.

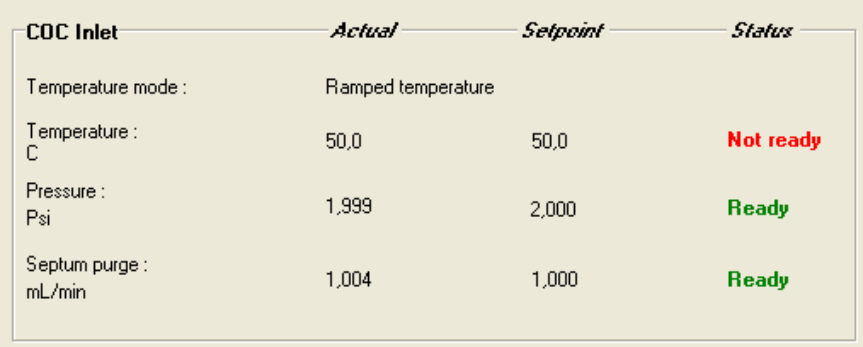
The actual and setpoint values of the Inlet Pressure are displayed. The pressure is the same than the one of the associated column.

The total flow is displayed.

The actual and setpoint values of the Inlet Septum purge are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

Cool on-column



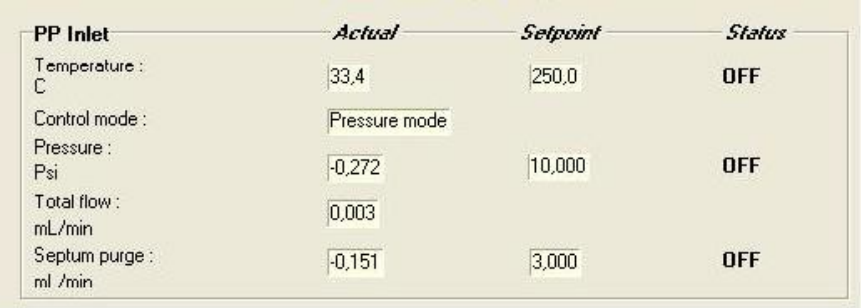
The actual and setpoint values of the Inlet Temperature are displayed.

The actual and setpoint values of the Inlet Pressure are displayed. The pressure is the same than the one of the associated column.

The actual and setpoint values of the Inlet Septum purge are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

Purged Packed inlet

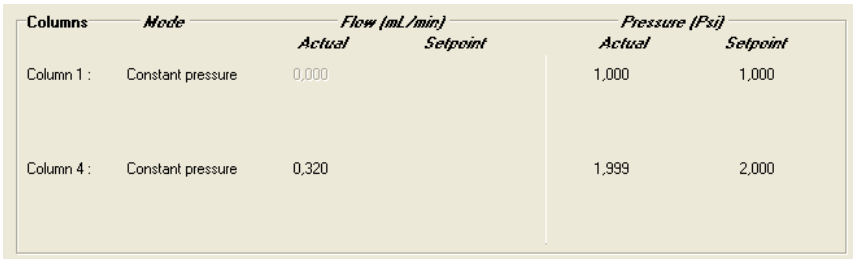


The actual and setpoint values of the Inlet Temperature are displayed. The control mode is displayed.

The actual and setpoint values of the Inlet Pressure are displayed.

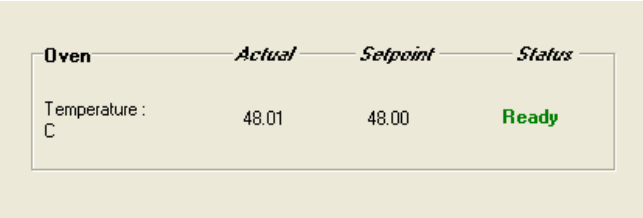
The actual and setpoint values of the Inlet Septum purge are displayed.

Columns:



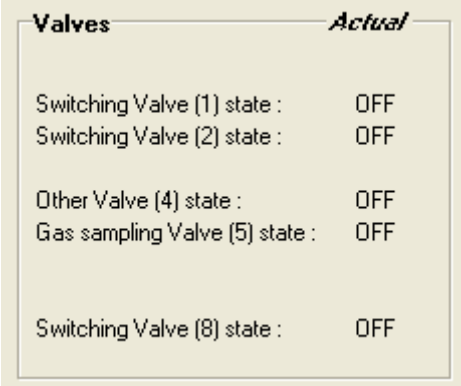
For each connected column, the Actual Flow and Pressure are displayed. Only the Setpoint (Flow or Pressure) defined in the method is displayed (Flow Setpoint if in Constant or ramped flow, Pressure Setpoint if in constant or ramped pressure).

Oven:



The current value of the temperature and the setpoint are displayed. The status (Ready / Not ready) is also displayed.

Valves:

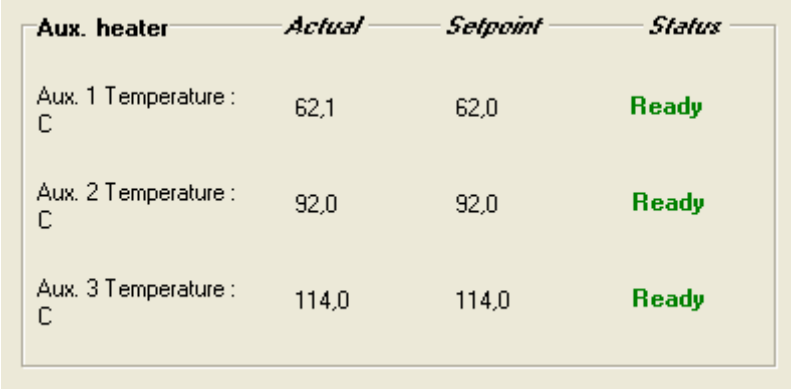

Valves
Actual
Switching Valve (1) state : OFF
Switching Valve (2) state : OFF
Other Valve (4) state : OFF
Gas sampling Valve (5) state : OFF
Switching Valve (8) state : OFF

The state (ON or OFF) of the valves is displayed in the status.

For *Gas Sampling Valve*, the state is OFF during the Load Time, and ON during the Inject Time period (both times values are defined in the method).

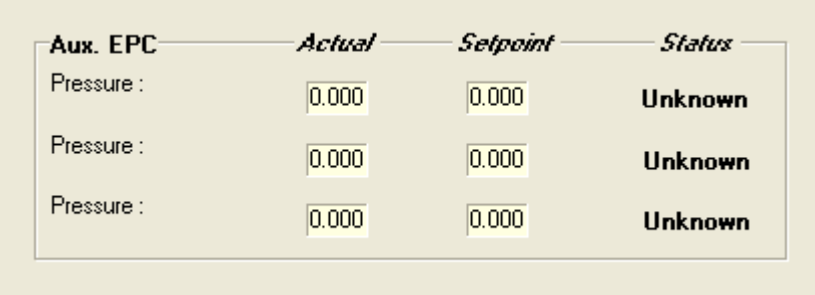
No information is displayed on the Multiposition valve.

Auxiliary Heater:



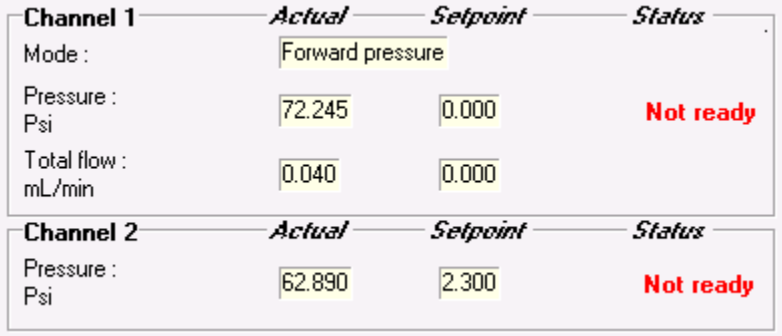
The current value of the temperature and the setpoint are displayed for each auxiliary heater. The status (Ready / Not ready) is also displayed.

Auxiliary Pressure Control (Aux EPC):



The current value of the pressure and the setpoint are displayed for each auxiliary pressure control. The status (Ready / Not ready/Unknown) is also displayed.

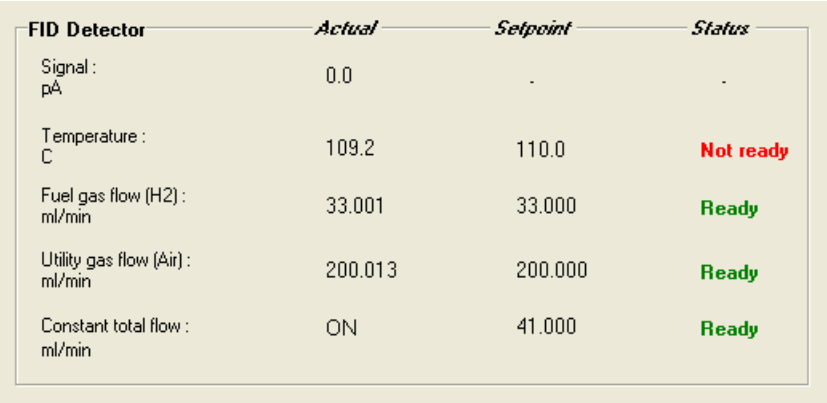
Pressure Control Module (PCM):



The current value of the pressure and the setpoint are displayed for each PCM channel. For channel 1 Flow setpoint and actual values are also displayed. The status (Ready / Not ready/Unknown/OFF) is precised.

Detectors:

FID



The current value of the signal is displayed in pA.

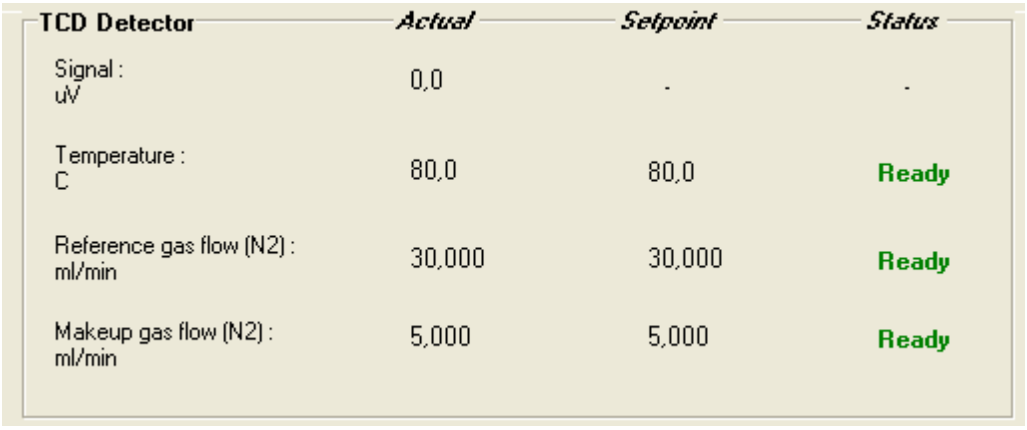
The actual and setpoint values of the detector Temperature, Fuel gas flow and Utility gas flow are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow has to be constant, this setting is ON, the setpoint value is displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow is not constant, the actual and setpoint values of the Makeup gas flow are displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method):

TCD



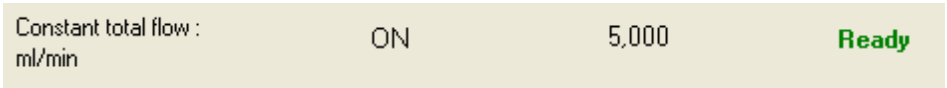
The current value of the signal is displayed in µV.

The actual and setpoint values of the detector Temperature, reference gas flow and make-up gas flow or Constant total flow are displayed.

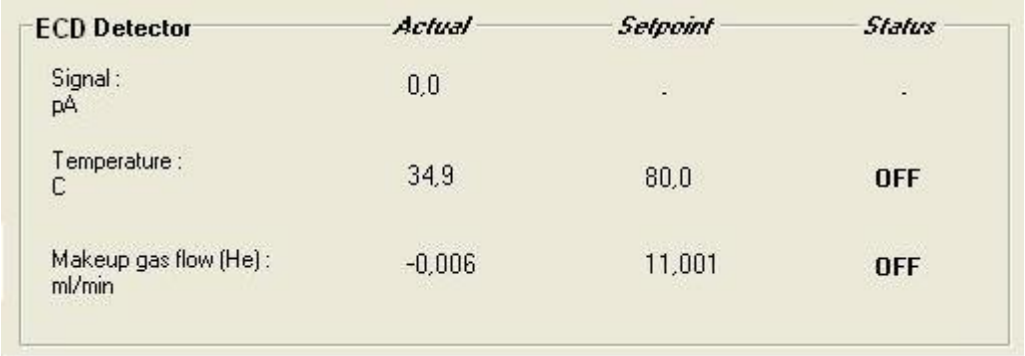
The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow has to be constant, this setting is ON, the setpoint value is displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow is not constant, the actual and setpoint values of the Makeup gas flow are displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is activated in the method):



ECD



The current value of the signal is displayed in pA.

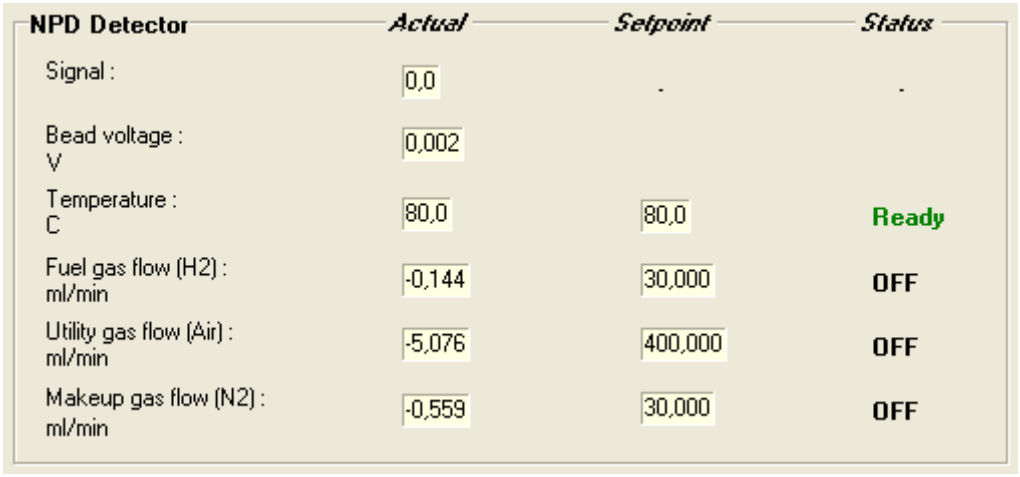
The actual and setpoint values of the detector Temperature and make-up gas flow or Constant total flow are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow has to be constant, this setting is ON, the setpoint value is displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow is not constant, the actual and setpoint values of the Makeup gas flow are displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is activated in the method):

NPD

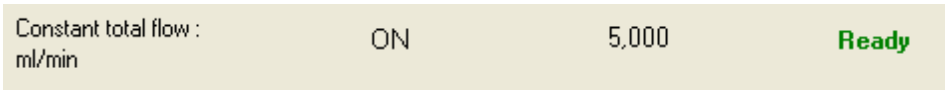


The current value of the signal is displayed.

The Bead Voltage actual value, the actual and setpoint values of the detector Temperature, Actual and setpoint Fuel gas flow and Utility gas flow are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow has to be constant, this setting is ON, the setpoint value is displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).



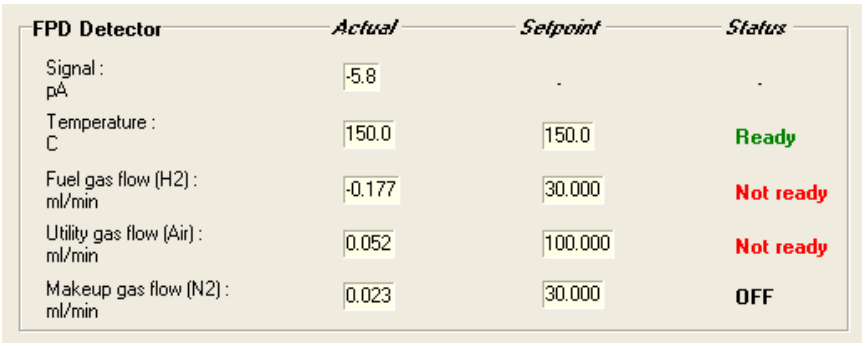
If the method specifies that the total flow is not constant, the actual and setpoint values of the Makeup gas flow are displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method):

Aux detectors

Aux detector 1 is necessarily a TCD , refer to the TCD section for status.

Aux detector 2 is necessarily an AIB. Only the signal value is displayed:

FPD



The current value of the signal is displayed in pA.

The actual and setpoint values of the detector Temperature, Fuel gas flow and Utility gas flow are displayed.

The status of each parameter is also clearly displayed. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow has to be constant, this setting is ON, the setpoint value is displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method).

If the method specifies that the total flow is not constant, the actual and setpoint values of the Makeup gas flow are displayed as well as its Status. It can be Ready / Not ready / Off (if the control of the parameter is not activated in the method):

Overview Window

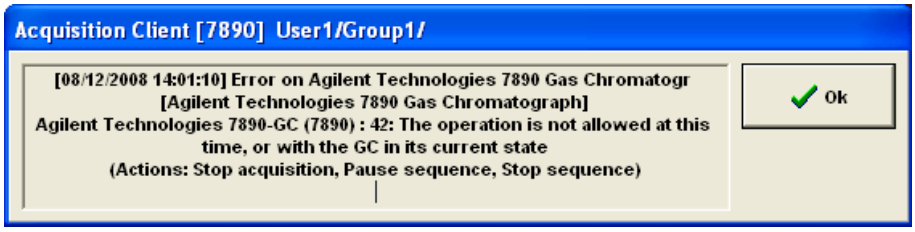
Click on the

button: for 7890 GC, nothing is displayed.

Troubleshooting

Error message when downloading a method

If the following error message is displayed during the download of a method:


Acquisition Client [7890] User1/Group1/
[08/12/2008 14:01:10] Error on Agilent Technologies 7890 Gas Chromatogr
[Agilent Technologies 7890 Gas Chromatograph]
Agilent Technologies 7890-GC (7890) : 42: The operation is not allowed at this time, or with the GC in its current state
(Actions: Stop acquisition, Pause sequence, Stop sequence)
Ok

It is because the 7890 is by default in “Auto Prep Run” mode. This prevents any download of CompassCDS methods, thus, any acquisition.

It is then required to change this setting.

To do so, on the GC, press the Config button and edit the Instrument menu. Change the setting of the Auto Prep Run parameter to Off.

Appendix

Injection Volumes

The volume injected depends on the Autosampler model (if one is controlled by CompassCDS).

If an Agilent 7683 autosampler (old model, until the G2913 turret) is present, the injection volume corresponds to syringe stops (1 to 6).

If an Agilent 7693 autosampler (new model, since the G4513 turret) is present, the injection volume will be entered in micro liters, and the available values will depend on the syringe size.

7683 autosampler model (G2613, G2913 turret)

	Value entered in the *Injection Volume* field of the acquisition method	Corresponding % of the syringe volume	Corresponding Injection volume (µL)
5 µL Syringe	1	2	0.1
	2	10	0.5
	3	20	1.0
	4	30	1.5
	5	40	2.0
	6	50	2.5
10 µL Syringe	1	2	0.2
	2	10	1.0
	3	20	2.0
	4	30	3.0
	5	40	4.0
	6	50	5.0
25 µL Syringe	1	2	0.5
	2	10	2.5
	3	20	5.0
	4	30	7.5
	5	40	10.0
	6	50	12.5
50 µL Syringe	1	2	1.0
	2	10	5.0
	3	20	10.0
	4	30	15.0
	5	40	20.0
	6	50	25.0
100 µL Syringe	1	2	2.0
	2	10	10.0
	3	20	20.0
	4	30	30.0
	5	40	40.0
	6	50	50.0

7693 autosampler model (G4513 turret)

	Value entered in the Injection Volume field of the acquisition method (µL)
5 µL Syringe	0 - 2.5
10 µL Syringe	0 - 5
25 µL Syringe	0 - 12.5
50 µL Syringe	0 - 25
100 µL Syringe	0 - 50
250 µL Syringe	0 - 125
500 µL Syringe	0 - 250

GC error codes

The following list translates the main error codes that can be returned by the 7890:

Error -1	unknown error";
Error 2	unspecified error";
Error 5	requested operation is not implemented on this port";
Error 6	string passed in the content of a request is too long";
Error 7	server (GC) has run out of memory";
Error 8	attribute or element value has the wrong format";
Error 9	buffer used to format a message is too small";
Error 10	value of an attribute or element is not in the valid range";
Error 11	server (GC) has too many subscribers to a given data/status/event";
Error 12	output message can't be sent";
Error 13	invalid pointer was passed to a function";
Error 14	required license key is not given";
Error 15	license key is not valid";
Error 16	license key does not grant sufficient rights";
Error 17	license key has expired";
Error 18	too many elements given";
Error 19	input message is too large for parser";
Error 20	an unsupported construct was used in a message";
Error 21	an element or attribute was duplicated";
Error 22	a string is not of the expected length";
Error 23	a string is too short";
Error 24	operation is not valid for this port";
Error 25	error parsing target url";
Error 26	internal error creating socket";
Error 27	target did not respond";
Error 28	target refused connection";
Error 29	GC refused to do an injection";
Error 30	GC refused to do a blank run";
Error 31	SubScribeToData:
Error 32	SubScribeToData:
Error 33	SubScribeToData:
Error 34	EEPROM device did not respond";
Error 35	EEPROM record address error";
Error 36	EEPROM device address out of range 0-9";
Error 37	EEPROM device did not respond correctly";
Error 38	Checksum error in EEPROM record";
Error 39	Client is not GC owner as required to perform command";
Error 40	SubscribeToData:
Error 41	ReadBarcode:
Error 42	The operation is not allowed at this time, or with the GC in its current state";

Autosampler error codes

The following list translates the main error codes that can be returned by the autosampler:

Error 100	Tray Z axis failed to find home.
Error 101	Tray Radius failed to find home.
Error 102	Tray Theta failed to find home.
Error 103	There was a bottle in the gripper.
Error 104	There was no bottle in the gripper.
Error 105	A stop key was pressed.
Error 106	The selected injector is not present.
Error 107	The tray is not present.
Error 108	Bar code reader is not present.
Error 110	Autoinjector communications error.
Error 111	Autoinjector front turret syringe error.
Error 112	Autoinjector front turret turret error.
Error 113	Autoinjector front turret plunger error.
Error 114	Autoinjector front turret incomplete injection.
Error 116	Autoinjector front door was open.
Error 117	Autoinjector front turret was reset.
Error 120	Autoinjector communications error.
Error 121	Autoinjector back turret syringe error.
Error 122	Autoinjector back turret turret error.
Error 123	Autoinjector back turret plunger error.
Error 124	Autoinjector back turret incomplete injection.
Error 126	Autoinjector back door was open.
Error 127	Autoinjector back turret was reset.

Agilent 7890 GC Control Driver Release Notes

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501586
Revision C

Introduction of the driver (4.0.0)

The Agilent 7890 GC CompassCDS control driver software requires CompassCDS version 3.0.1 or above (the CompassCDS versions 2.0 and 3.0 are not supported).

The Agilent 7890 GC can be controlled, via Ethernet, by CompassCDS software if the GC has the following firmware versions:

- 7890A GC: A.01.12; A.01.12.1; A.01.15.2
- 7890B GC: B.02.00; B.02.02

Supported configurations

- Inlets:

  Split/splitless capillary inlet (S/SL)

  Temperature-programmable cool on-column inlet (PCOC)

  Purge Packed inlet (PP)

  Multi Mode inlet (MMI)

- Detectors:

  Flame ionization detector (FID)

  Thermal conductivity detector (TCD)

  Electron capture detector (ECD)

  Nitrogen Phosphorous detector (NPD)

  Flame Photometric detector (FPD)

- Autosampler:

  Automatic liquid sampler (ALS) type 7683 (G2913A and G2613A) including the 100 vials tray

  Automatic liquid sampler (ALS) type 7693 (G4513A) including the 150 vials tray (G4514A)

  The Standard, Sandwich injection and Large Volume injection (LVI) modes are supported with the 7693 Autosampler

- The Oven Cryogenic coolant is controlled
- PCM (Pressure Control Module) is controlled
- Multi injector, multi detector: CompassCDS can control any 2 auto sampler, 2 Inlet, 2 detector configuration as long as the configuration consists of the elements described above.
- Valves. Eight valves can be controlled. Among them we support the Gas Sampling valve, the Switching valve and the Multi-position valve.

- Aux detector 1 (TCD) and Aux detector 2 (AIB) are supported (see Known problems part below about the auxiliary detectors.)
- Auxiliary heaters. Three auxiliary heaters can be controlled, among the ones proposed by the GC (AED transfer line, user configurable, Nickel Catalyst, etc.).
- The Auxiliary EPCs are controlled
- The Gas saver option working with a manual injector
- Run time events.

Known issues

- The 1µL syringe is not supported due to a CompassCDS core defect.
- If the syringe size is changed in the GC, the user needs to exit CompassCDS session, and then to enter in the system configuration for the software to pick up the new syringe size, and then, stop/start the system.

  Moreover, new methods that match the new syringe size limits of the injection volume field in the acquisition part of the method will need to be created.
- The BEAD Voltage parameter is controlled by the driver for the NPD detector. The value has to be set on the GC itself.
- If adding auxiliary detector(s) to an existing system, new channel(s) will be automatically declared in CompassCDS Configuration Manager. The previous methods (created on the previous system configuration) will no longer be compatible, as a method is created for a system with a defined number of channels. To use those methods the new channels must be disconnected from within the CompassCDS Configuration Manager.

CompassCDS
Agilent 1260 LC Driver
User Guide

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501611
Revision A

Contents

Introduction 3
Installation and Configuration 4
  Installing the Driver Software 4
  Configuring the HPLC Communications 4
  Configuring the Driver 7
Building a Method 23
  Creating a New Method 23
  Control Method Section for the Agilent Technologies 1260 Modules 25
Starting and Viewing an Acquisition 70
  Quick Start and Sequence 70
  Running Acquisition Status 71
Running Instrument Maintenance Software 102
  Software Presentation 102
  Software Functions 102
  Performing Maintenance and Diagnosis 103
  Diagnostic Section for the Agilent Technologies 1260 Modules 103
  Reporting Maintenance Audit trail 124
Appendix 127
  GPIB Addresses 127
  Configuring a Fixed IP Address 128

Introduction

This document describes the configuration of the Agilent Technologies 1260 LC Modules drivers. It also explains how to build a control method for these drivers, how to start and view a running acquisition, what actions are available during an analysis and how to diagnose using the Instrument Maintenance Software.

This driver supports different modules from:

- Agilent Technologies 1100 LC series
- Agilent Technologies 1200 LC series
- Agilent Technologies 1260 LC series

The supported modules are:

- Isocratic Pump (G1310)
- Quaternary Pump (G1311)

  Also controls the Bio-Inert Quaternary pump G5611
- Binary Pump (G1312)
- AutoSampler (G1313)
- Variable Wavelength Detector (G1314)
- Diode Array Detector (G1315)

  Also controls the Multiple Wavelength detector (G1365)

  Also controls the Diode Array Detector (G4512)
- Column Compartment (G1316)
- Fluorescence Detector (G1321)
- Thermostated AutoSampler (G1329)
- Refractive Index Detector (G1362)
- Well Plate Autosampler (G1367)

Installation and Configuration

Installing the Driver Software

The CompassCDS software must already be installed before installing the driver software (refer to the CompassCDS Installation Guide).

Configuring the HPLC Communications

Serial Communications

Configuring the communication server

To communicate with the Agilent 1260 modules, a GPIB_Interface or an NI488 communication bus must be configured on the acquisition server.

To communicate with the modules, the buffer parameters of the GPIB_Interface bus must be the following:

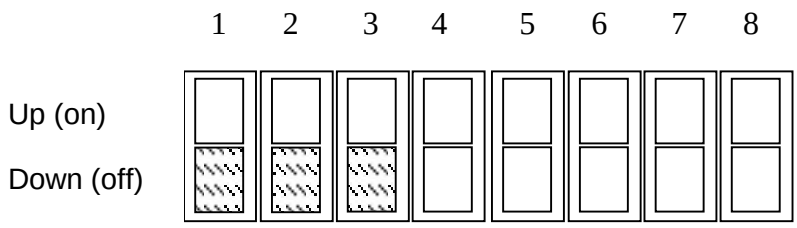
- TX Buffer: 1024
- RX Buffer: 5120

NOTE: For more details about the configuration of a GPIB_Interface or an NI488 bus, refer to the CompassCDS Installation Guide.

Connecting the Agilent LC 1260 modules to CompassCDS

The CompassCDS Chromatography Data System uses GPIB to communicate with the Agilent 1260 modules.

For each Agilent 1260 module controlled by CompassCDS, a switch located on the rear panel of the instrument must be configured appropriately. For all the modules, the first three switches from left must be turned off (Down Position) for control with CompassCDS as for control with HP-CHEMSTATION. Changing the position of these switches must be done with module switched-off.



The module where the GPIB cable is connected should be the detector of the HPLC chain (as recommended by Agilent). This module is called the Master module. The rest of the modules of the HPLC chain communicate through the Master module via CAN cables. The GPIB address entered in each module in the CompassCDS Configuration Manager must be the GPIB address of the master module.

Ethernet Communications

The Agilent Technologies 1260 LC modules can use Ethernet ® as the method of communications for instrument control and for sending digital data to the external data system. Ethernet communication is not standard on the Agilent 1260 LC. The Ethernet connection is made at the back of the 1260 LC. There are two types of Ethernet cables:

- An Ethernet crossover cable is used when the Agilent 1260 LC is connected directly to the CompassCDS Acquisition Server PC.
- A standard Ethernet patch cable is used when the Agilent 1260 LC is connected to a company Ethernet network.

The Agilent 1260modules uses TCP/IP (Transmission Control Protocol / Internet Protocol) to communicate over the Ethernet network and needs to be given a unique IP address to identify the instrument.

A BOOTP Server or a DHCP server is used to send IP addresses to TCP/IP devices.

The BOOTP Server lists Ethernet addresses along with the IP addresses that are to be assigned to the corresponding devices.

Configuration for the BOOTP server, is in the CompassCDS installation Guide.

It is also possible to give a fixed IP address to the Agilent 1260 LC. For information on how to fix the IP address of the Agilent 1260 LC, refer the appendix: Configuring a Fixed IP Address in this manual.

NOTE: The BOOTP server provided by CompassCDS is installed during the installation of the CompassCDS software.

It is advised to set the IP address as a fixed IP address.

Following are examples of connections between CompassCDS and Agilent 1260 modules.

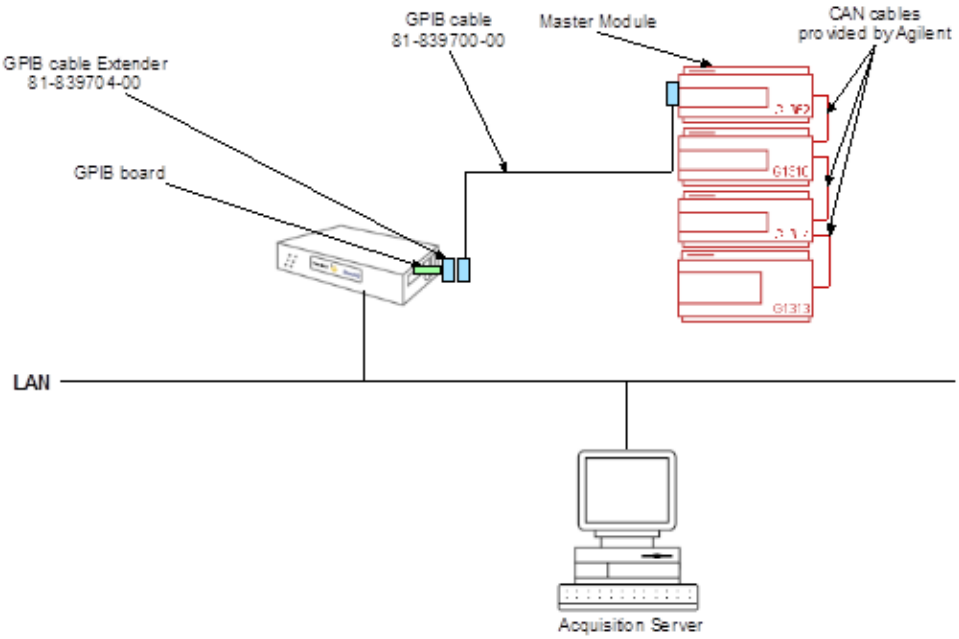


Figure 1 Agilent 1260 connected to an MIB-interface with a GPIB board

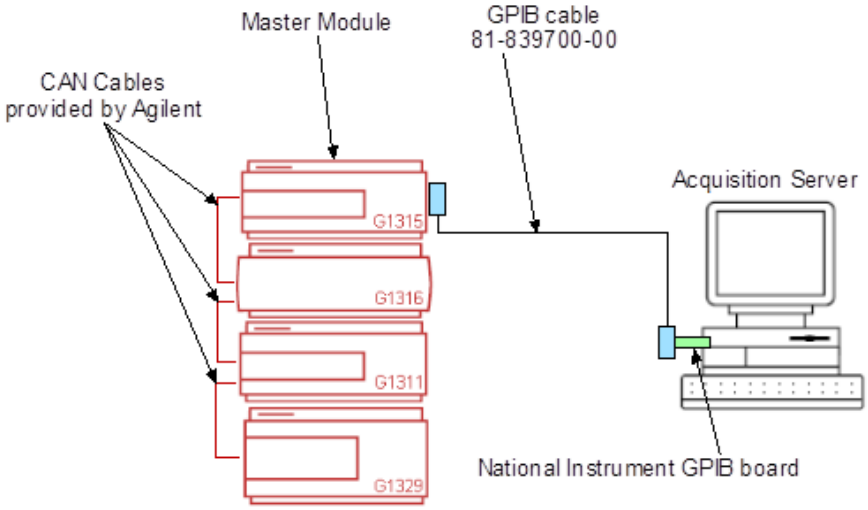


Figure 2 Agilent 1260 connected to an NI GPIB board

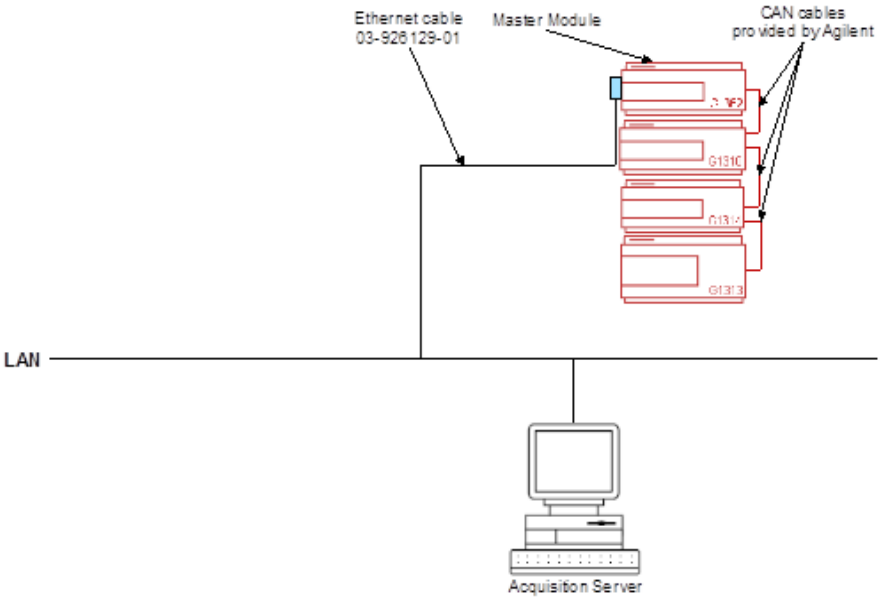


Figure 3 Agilent 1260 connected to an Ethernet cable

Configuring the Driver

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

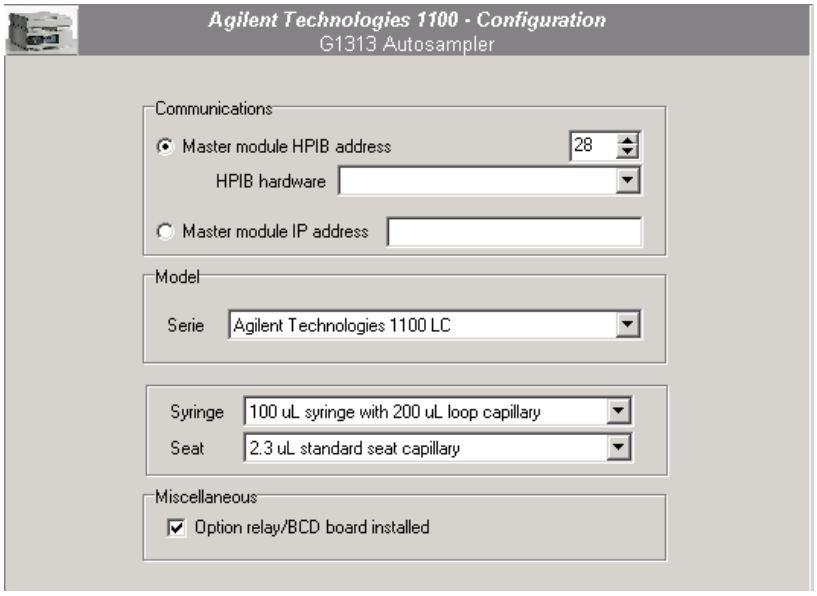
Configuring the Agilent Technologies LC 1260 AutoSamplers

The Agilent Technologies 1260 AutoSampler (G1313), the Agilent Technologies 1260 Thermostated AutoSampler (G1329), and the Agilent Technologies 1260 Well Plate AutoSampler (G1367) are available.

Click on the

button corresponding to the Agilent Technologies 1260 Autosampler driver and the configuration screen appears.

For the G1313 and G1329 modules, the following screen is displayed:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

In the Syringe scrolling list, select the injector syringe type. Two choices are available: 100 µL syringe with 200 µL loop capillary and 900 µL syringe with 1800 µL loop capillary.

In the Seat scrolling list, select the seat type. Five choices are available: 2.3 µL standard seat capillary, 1.2 µL low dispersion and 800 µL, 2800 µL and 8000 µL seat capillary for multiple draw.

Model Group

Choose the LC model according to the LC type installed. Select Agilent Technologies 1100 LC or Agilent Technologies 1200 LC or Agilent Technologies 1260 LC according to the LC type installed

Syringe Group

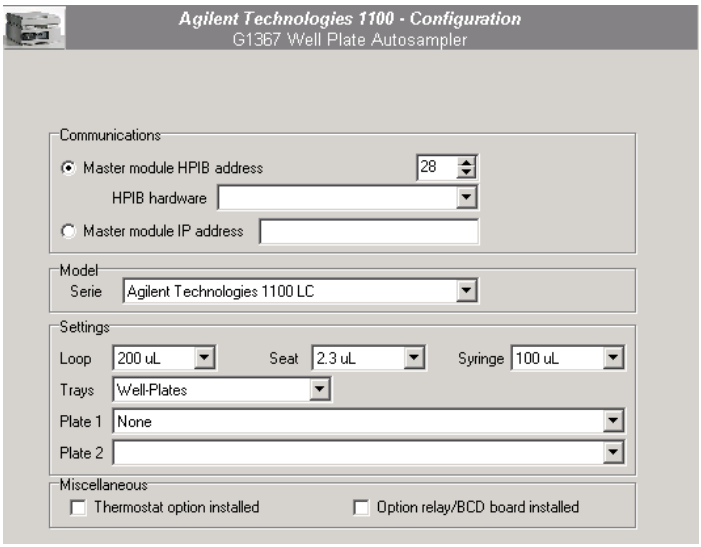
In the Syringe size scrolling list, select the syringe type. Two choices are available: 100 µL with 200 µL loop capillary or 900 µL with 1800 µL loop capillary.

In the Seat *capillary* scrolling list, select the seat type. Five choices are available: 2.3 µL standard seat capillary, 1.2 µL low dispersion, 800 µL seat capillary for multiple draw, 2800 µL seat capillary for multiple draw, 8000 µL seat capillary for multiple draw.

Miscellaneous Parameter Group

Check the Option relay/BCD board installed if a relay board is installed on the module.

For the G1367 module, the following screen is displayed:



Following is a table for possible values and the field limits corresponding to these settings. Please note that the driver does not detect an incorrect setting, but the module will enter a line in the logs if an incorrect setting is detected.

Product	Syringe (µL)	Seat capillary (µL)	Loop capillary (µL)	Min speed µL/min	max draw speed µL/min	max eject speed µL/min	max rinse speed µL/min
G1367 D	40	1.15	102	4	1000	1000	1000
	40	2.30	102	4	1000	1000	1000
	40	400	102	4	1000	1000	1000
G1367 E	40	1.15	80	4	1000	1000	1000
	40	2.30	80	4	1000	1000	1000
	40	400	80	4	1000	1000	1000
G1367 A-E	100	1.15	200	10	1000	1000	2500
G1367 D	100	2.30	200	10	1000	1000	2500
G1367 A-C, G1367 E	100	2.30	200	10	1000	1000	2500
G1367 A-E	100	400	200	10	1000	1000	2500
	100	1400	200	10	1000	1000	2500
	100	5000	200	10	1000	1000	2500
G1367 A-C	900	1.15	1800	90	1000	1000	2500
	900	2.30	1800	90	1000	1000	2500
	900	400	1800	90	1000	1000	2500
	900	1400	1800	90	1000	1000	2500
	900	5000	1800	90	1000	1000	2500

Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Choose the LC model according to the LC type installed. Select Agilent Technologies 1100 LC or Agilent Technologies 1200 LC or Agilent Technologies 1260 LC according to the LC type installed

Settings Parameter Group

In the Syringe size scrolling list, select the syringe type. Four choices are available: 8 µL, 40µL, 100 µL or 400 µL.

In the Seat capillary scrolling list, select the seat type. Seven choices are available: 0.3 µL, 0.7 µL, 1.2 µL, 2.3 µL, 400 µL, 1400 µL or 5000 µL.

In the Loop capillary scrolling list, select the Loop type. Four choices are available: 8 µL, 80 µL, 200 µL and 1800 µL.

In the Trays scrolling lists, select the type of trays installed in the autosampler. Five choices are available: None, 15 vials, 40 vials, 100 vials and Well Plate.

In the Plates X scrolling lists, select the type of plates installed in the Well Plate tray.

NOTE: Only *96Agilent* and *384Agilent* plates are controlled.

Miscellaneous Parameter Group

Check the Thermostat Option installed check box if the autosampler is thermostated.

Check the Option relay/BCD board installed check box if a relay board is installed on the module.

Configuring the Agilent Technologies LC 1260 Pumps

The Agilent Technologies 1260 Isocratic Pump (G1310), the Agilent Technologies 1260 Quaternary Pump (G1311) and the Agilent Technologies 1260 Binary Pump (G1312) are available.

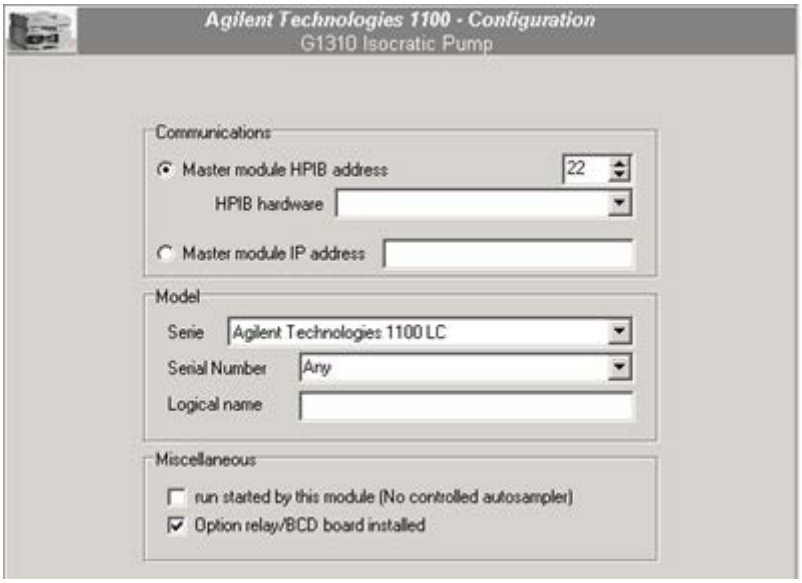
Click on the

,

or

button according to the pump type to display the configuration screen.

For the G1310, the following screen is displayed:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Choose the LC model according to the LC type installed.

If you are using several G1310 isocratic pumps on the same system, you need to install several times the driver and enter each pump serial number into the field Serial Number. If a single pump is installed, you'd better let ANY.

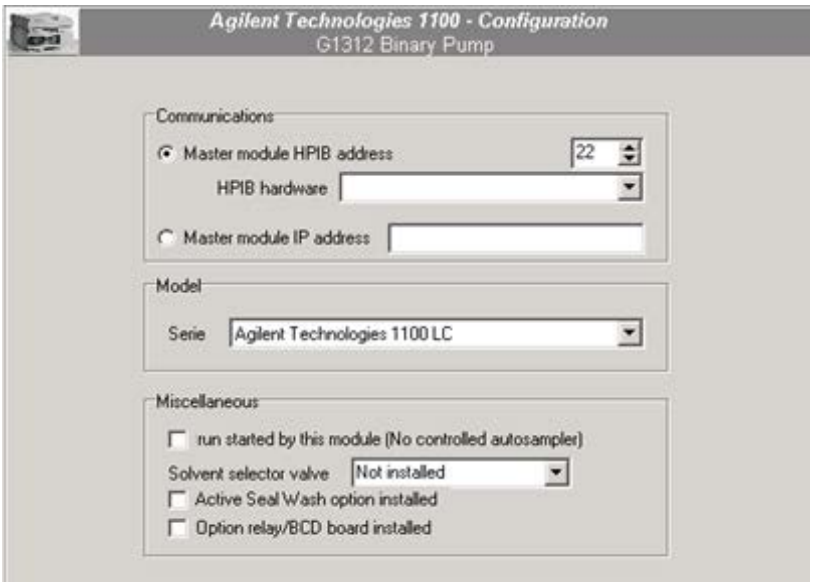
You can give a logical name to the pump. This name will be displayed into the second line of each screen title to avoid confusion between the different pumps (This is mainly useful in multiple pumps configurations).

Miscellaneous Parameter Group

Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260 module. The CompassCDS run will start as soon as this module is started.

Check the Option relay/BCD board installed check box if a relay board is installed on the module.

For the G1312 module, the following screen is displayed:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Choose the LC model according to the LC type installed.

Miscellaneous Parameter Group

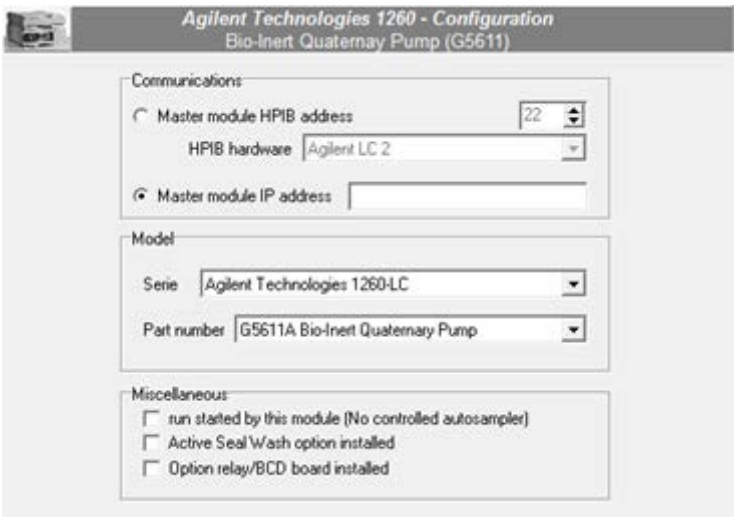
Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260 module. The CompassCDS run will start as soon as this module is started.

Solvent selector valve: Choose Installed if a solvent selection valve is installed. The solvent selection valve (optional) permits selecting a binary mixture (isocratic and gradient) from four independent solvent bottles.

Check the Active Seal Wash box if the Active Seal Wash option is installed on the pump. In order to preserve the seal, the seal wash option permits washing the back side of the seal.

Check the Option relay/BCD board installed check box if a relay board is installed on the module.

For the G1311 and G5611 modules, the following screen is displayed:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and then type the IP address of the instrument.

Model Group

Serie

Choose the LC model according to the LC type installed. Select Agilent Technologies 1100 LC, Agilent Technologies 1200 LC or Agilent Technologies 1260 LC according to the LC type installed

Part number

Select the module type. Two choices are available: G1311A/B (for Standard Quaternary pump) or G5611A (for Bio-Inert quaternary pump).

Miscellaneous Parameter Group

Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260 module. The CompassCDS run will start as soon as this module is started.

Check the Active Seal Wash box if the Active Seal Wash option is installed on the pump. In order to preserve the seal, the seal wash option permits washing the back side of the seal.

Check the Option relay/BCD board installed check box if a relay board is installed on the module.

Configuring the Agilent Technologies 1260 LC Column Compartment

Click on the

button to display the configuration screen:

Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Choose the LC model according to the LC type installed.

Miscellaneous Parameter Group

Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260 module. The CompassCDS run will start as soon as this module is started.

Hardware Parameter Group

Check the Switch valve option installed check box if a switch valve is present in the module.

Configuring the Agilent Technologies LC 1260 Detectors

The Agilent Technologies 1260 Variable Wavelength Detector (G1314), the Agilent Technologies 1260 Diode Array Detector (G1315), the Agilent Technologies 1260 Fluorescence Detector (G1321) and the Agilent Technologies 1260 Refractive Index Detector (G1362) are available. Choose the Agilent Technologies 1260 Diode Array Detector (G1315) to drive the Agilent Multiple Wavelength Detector (G1365) and the G4212B Diode Array Detector for Agilent 1260 Infinity LC.

Click on the

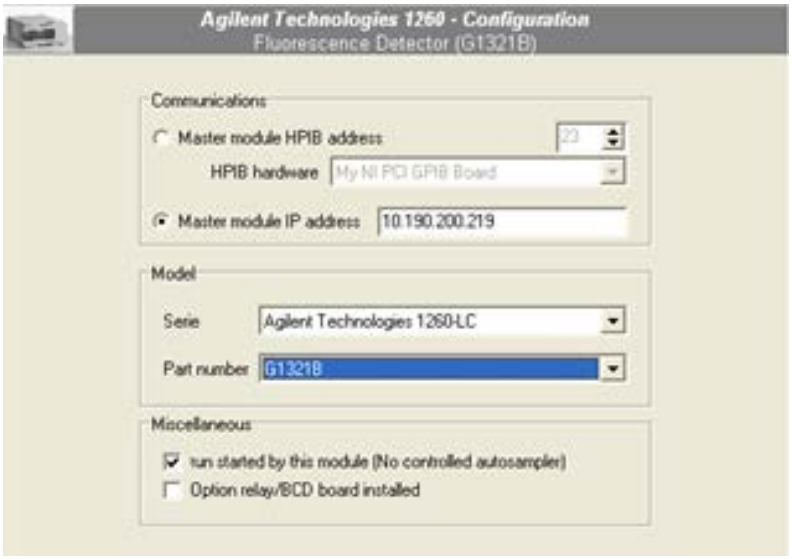
or

or

or

button according to the detector type to display the configuration screen.

The same screen is displayed for the G1362 and G1321 modules:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Serie

Select the LC model according to the LC type installed: Agilent Technologies 1100 LC, Agilent Technologies 1200 LC, or Agilent Technologies 1260 LC.

Part Number

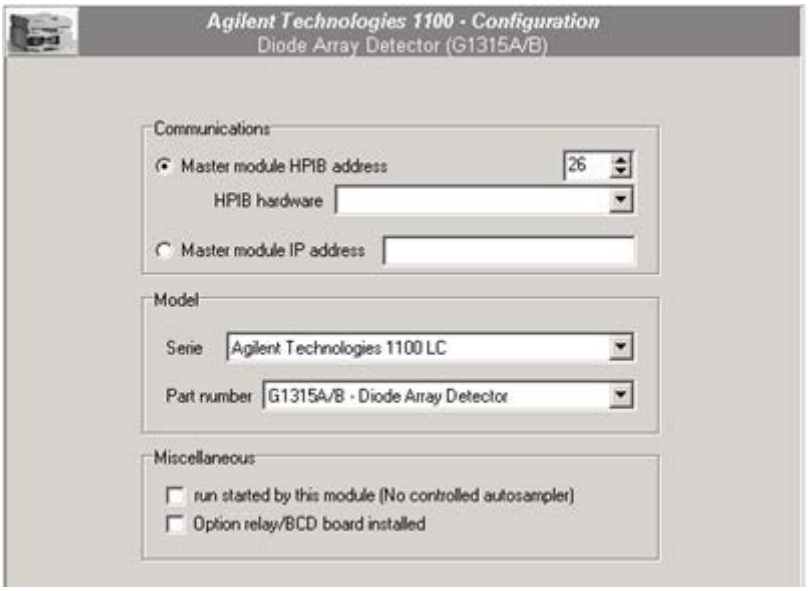
Select the module type. Two choices are available: G1321B (for FLD with spectra and multi-signal capabilities) or G1321C (for FLD without spectra and multi-signal capabilities).

Miscellaneous Parameter Group

Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260module. The CompassCDS run will start as soon as this module is started.

Check the Option relay/BCD board installed check box if a relay board is installed on the module.

The same screen is displayed for the G1315 and G1314 modules:



Communications Parameter Group

Master module HPIB Address:

Select this option if the HPLC chain is controlled via a GPIB communication and enter the GPIB address of the Master module.

NOTE: To check the GPIB address value of the Master module, refer to the Appendix at the end of this manual.

HPIB Hardware:

If the HPLC chain is controlled via a GPIB communication, select the name of the bus previously configured in the HPIB Hardware scrolling list.

NOTE: For more details about the Bus configuration, refer to the Configuring the Communication Server section in this manual.

Master module IP Address:

Select this option if the chromatograph is controlled via Ethernet communication and type the IP address of the instrument.

Model Group

Serie

Select the LC model according to the LC type installed. (Agilent Technologies 1100 , 1200 or 1260 LC) and the G4212B Diode Array Detector for Agilent 1260-LC

Part Number

Select the module type.

Seven choices are available for the G1315/G1365/G4212 modules: G1315A/B-DAD; G1365A/B-MWD; G1315C-DAD; G1365C- MWD, G1315D-DAD; G1365D-MWD; G4212B-DAD (Agilent Technologies 1260-LC module).

Five choices are available for the G1314 module: G1314A/B; G1314C (Fast); G1314D; G1314 E (Fast); G1314 F (Agilent Technologies 1260-LC module).

Miscellaneous Parameter Group

Check or uncheck the CompassCDS run started by this module (No controlled autosampler) check box. This box should be checked if a non-controlled autosampler present in the system is cabled to this module to give a start signal to the 1260 module. The CompassCDS run will start as soon as this module is started.

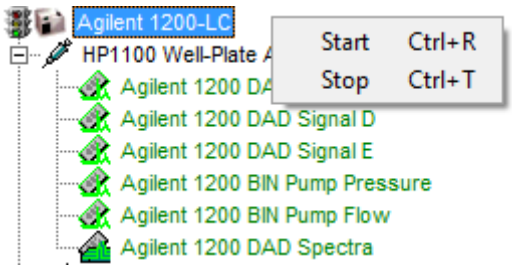
Check the Option relay/BCD board installed check box if a relay board is installed on the module.

Configuring the Synopsis

In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

1. To save the configuration of these devices, click on the OK button.

2. Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

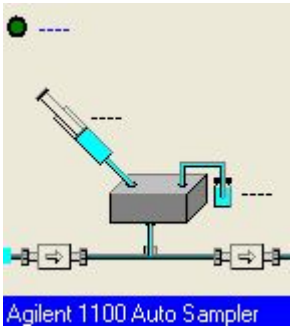


3. Go back to the System Configuration screen. A graphic of the devices that comprise the system is displayed in the synopsis screen. To configure the synopsis as the real instrument configuration, move each module, and then connect it appropriately. To do this, select one anchor for each of the two modules (the selected anchors become red) and click on the button; a connection tube will appear between the two anchors.

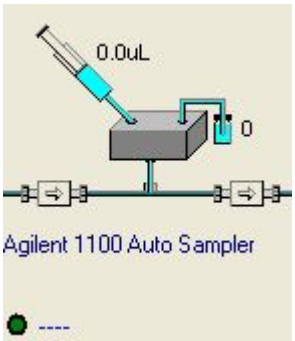
   Click on the to delete a selected tube, click on the buttons to delete all the tubes. Click on to define a background color, or on to make the background transparent. Click on the icon to change the grid color.

4. Once the synopsis configuration is complete, it will be displayed in the CompassCDS Chromatography Data System, in the *Systems* tab. In this tab, the *Overview* part will show the synopsis of the system with some parameters displayed (temperature, flow, signal, etc.) depending on the installed devices.

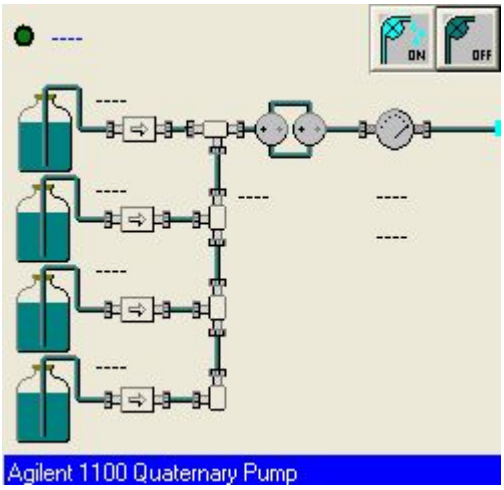
   For example, the following pictures represent the synopsis of the Agilent Technologies 1260modules:



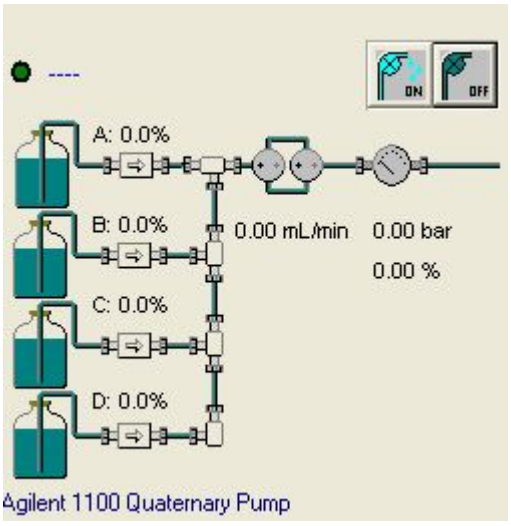
Agilent 1260 autosampler CompassCDS Configuration Manager Screen



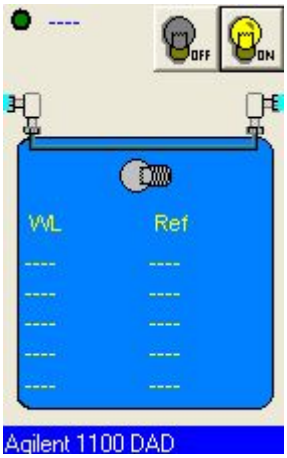
Agilent 1260 autosampler CompassCDS Chromatography Data System Screen



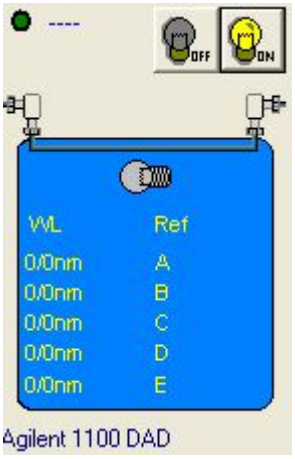
Agilent 1260 pumps CompassCDS Configuration Manager Screen



Agilent 1260 pumps CompassCDS Chromatography Data System Screen



Agilent 1260 detectors CompassCDS Configuration Manager Screen



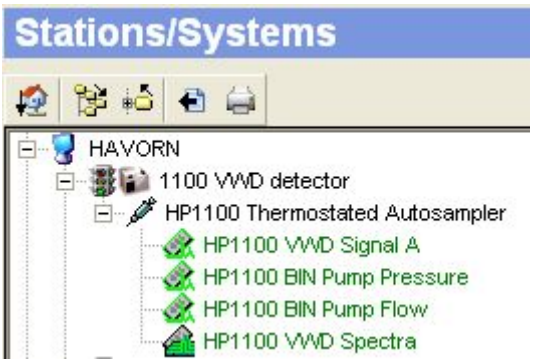
Agilent 1260 detectors CompassCDS Chromatography Data System Screen

Signal Configuration

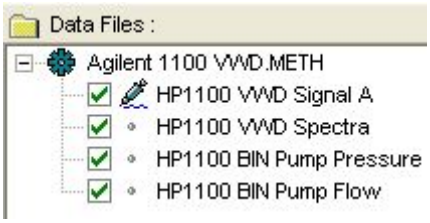
With all the detectors except with the Agilent Technologies 1260 Refractive Index Detector, it is possible to use several channels, up to six chromatographic signals with the Agilent Technologies 1260 Diode Array Detector G1315 or the Agilent Technologies 1260 Diode Array Detector G4212.

The example given below for the Agilent Technologies 1260 Diode Array Detector G1315 explains how to disconnect channels. The procedure is the same for all detectors.

In the Configuration Manager, the system is displayed as shown below:

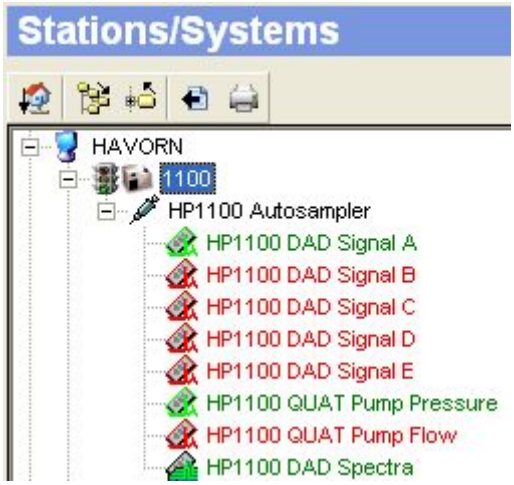


The method created on this system will have the following structure:



However, if some of these signals are NEVER used, it is possible to disconnect them.

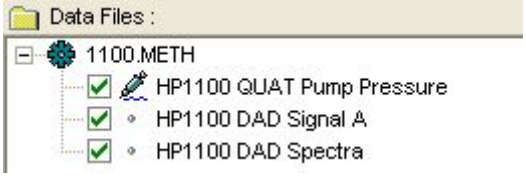
For instance, in the CompassCDS Configuration Manager, a system has the following configuration:



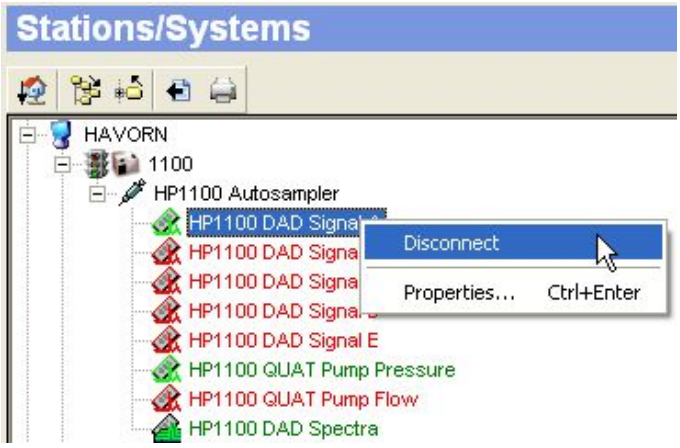
The icon indicates that the corresponding channel is activated.

The icon indicates that the corresponding channel is deactivated.

The methods created on this system will have the following structure:



1. To deactivate a channel, right click on the channel and select Disconnect in the pop-up menu:



2. Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration (not applicable to this driver).

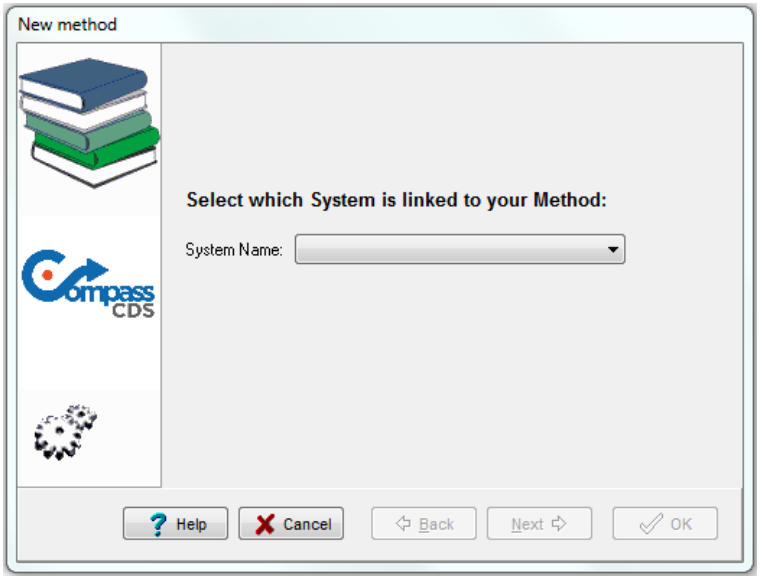
Building a Method

Creating a New Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and editing of final results. To initially set up a method, it is not necessary to define all of the sub-method sections; however, you must fill in the instrument control section prior to starting an acquisition.

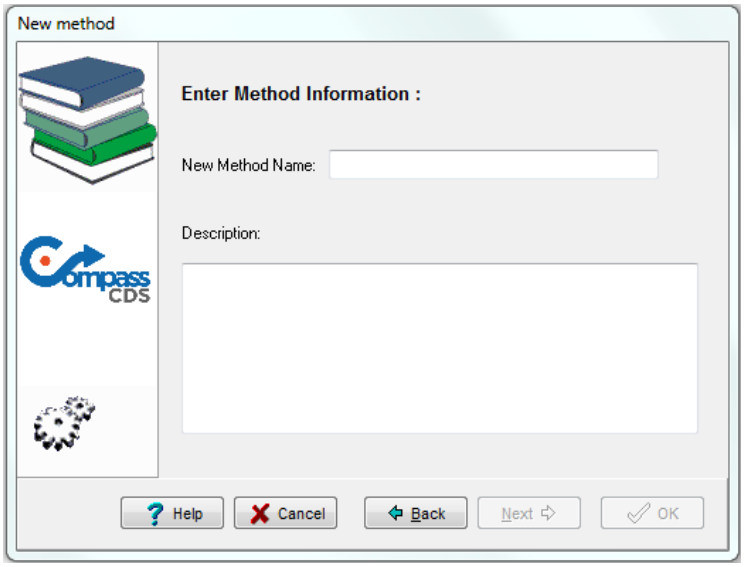
1. To create a new method, select the FILE / NEW METHOD option from the CompassCDS Chromatography Data System main menu.

   A wizard guide will appear and provide assistance during the first steps of method creation:



2. Choose the system (chromatograph) associated with the method. A method is created for a particular system. When starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those methods associated with this system.

3. Once this field is completed, click on the Next button to move to the second step of the method creation:



4. Enter the New Method Name in the first field. In the Description field, enter information concerning the method (optional).

5. Once these two fields have been completed, click on the OK button. The new method is created and is opened with default parameters in the CompassCDS Chromatography Data System. The next step is the definition of each of the method sections.

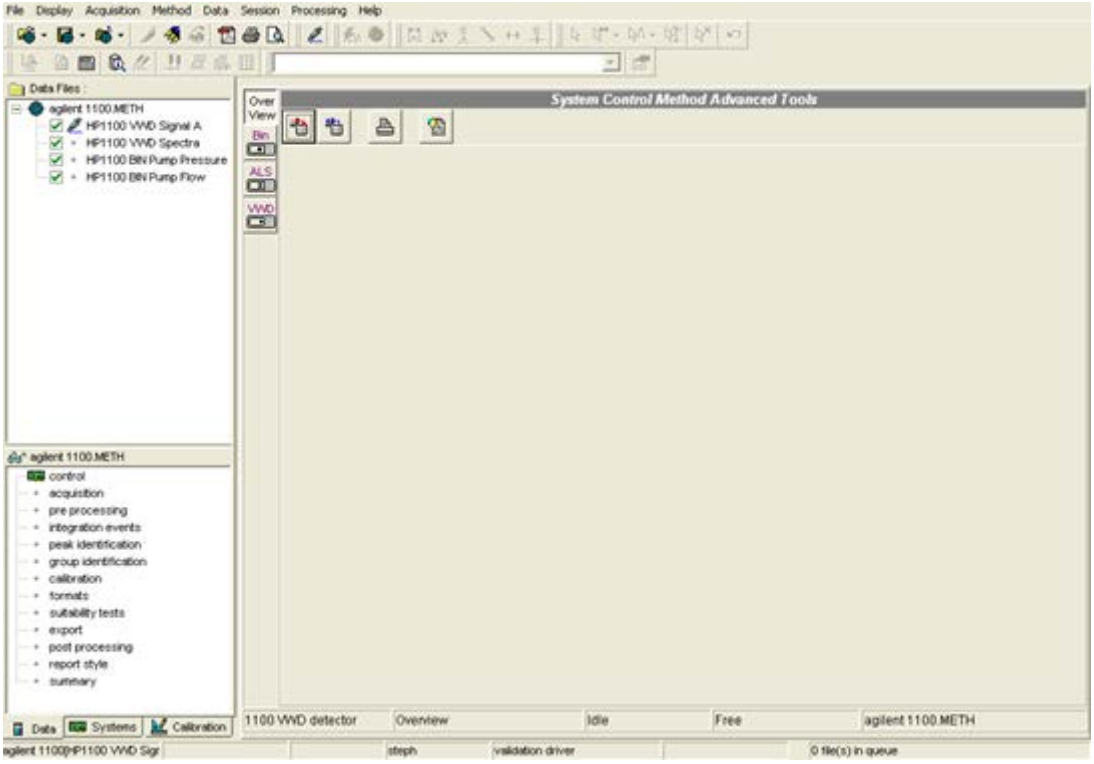
   The control section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the Agilent Technologies 1260LC Modules is detailed. Other parameters such as Injection Volume, Vial and Rack number may be necessary and are defined in the acquisition section.

NOTE: For more details about the programming of each method section, turn to the CompassCDS User Guide.

Control Method Section for the Agilent Technologies 1260 Modules

Once the new method is created, select the control section in the lower part of the browser.

The following screen appears:



Press the Over View button to display the ***System Control Method Advanced Tools*** window:

to send the current method to the instrument

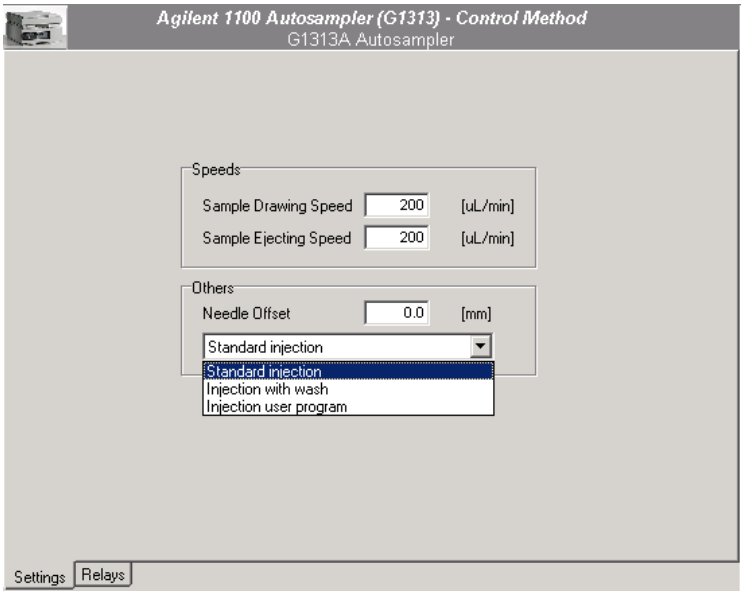
to get the active method from the instrument
(not applicable to these drivers)

to print the current method

Control Section for the Agilent 1260 AutoSampler (G1313)

Click on the

button to display the Agilent Technologies 1260 AutoSampler (G1313) control method section and to define the corresponding parameters that will be used during the chromatographic run.



Settings tab

Speeds Parameter Group

In the Sample Drawing Speed field, enter the sample aspiration speed value.

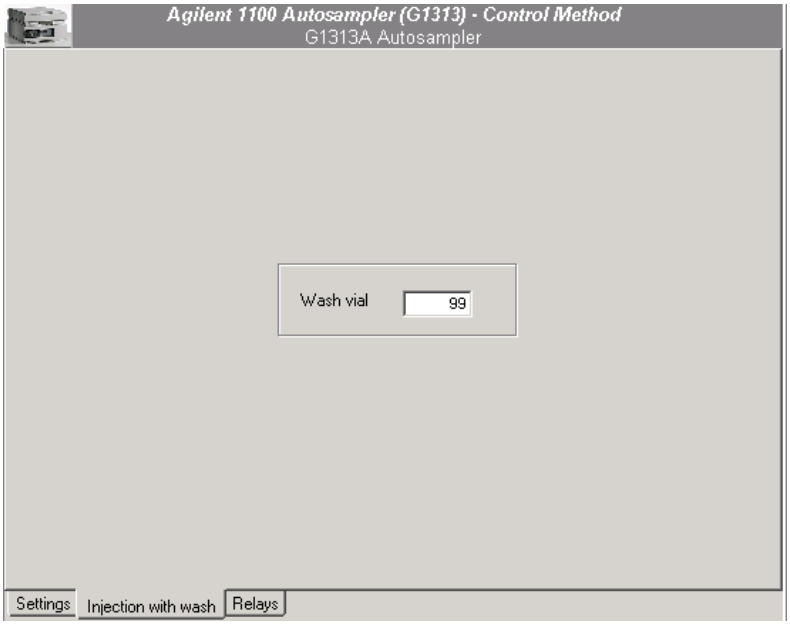
In the Sample Ejecting Speed field, enter the sample injection speed value.

Others Parameter Group

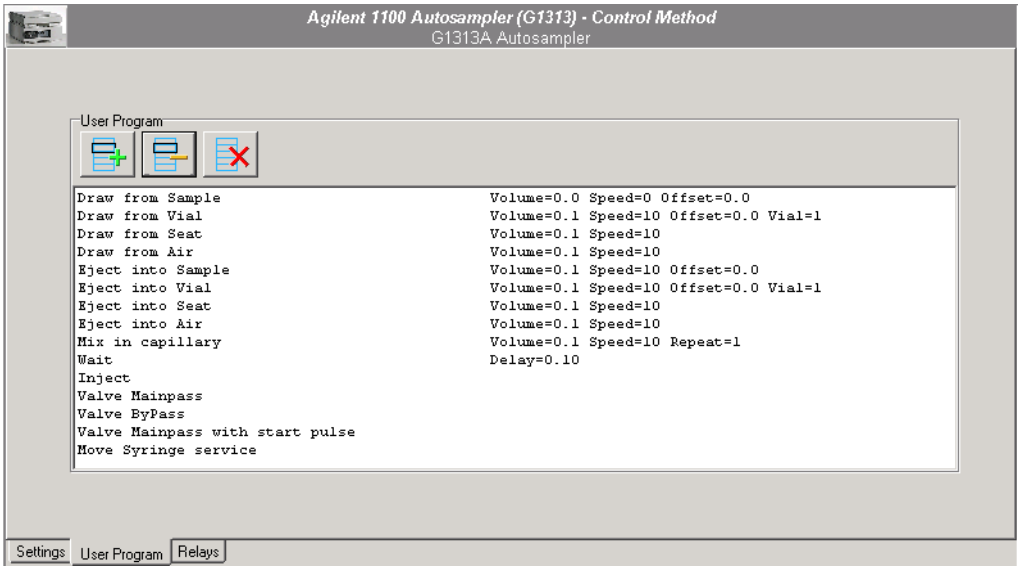
In the Needle Offset field, enter the vertical needle offset value.

Select the injection mode in the scrolling list. Three choices are available: Standard injection, Injection with wash and Injection user program.

- Standard injection: only the default screen is displayed. No other parameters are displayed.
- Injection with wash: when selecting this injection mode, another tab is displayed allowing the user to define the Wash vial.



- Injection user program: when selecting this injection mode, another tab is displayed allowing you to program different actions.



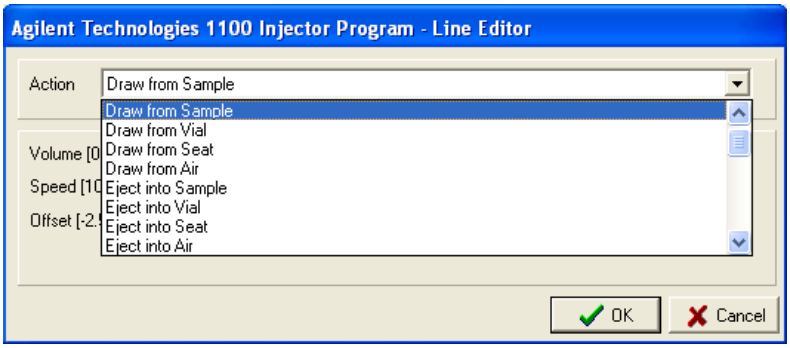
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

After a new line has been added, double-click on it to edit. A new window is displayed:



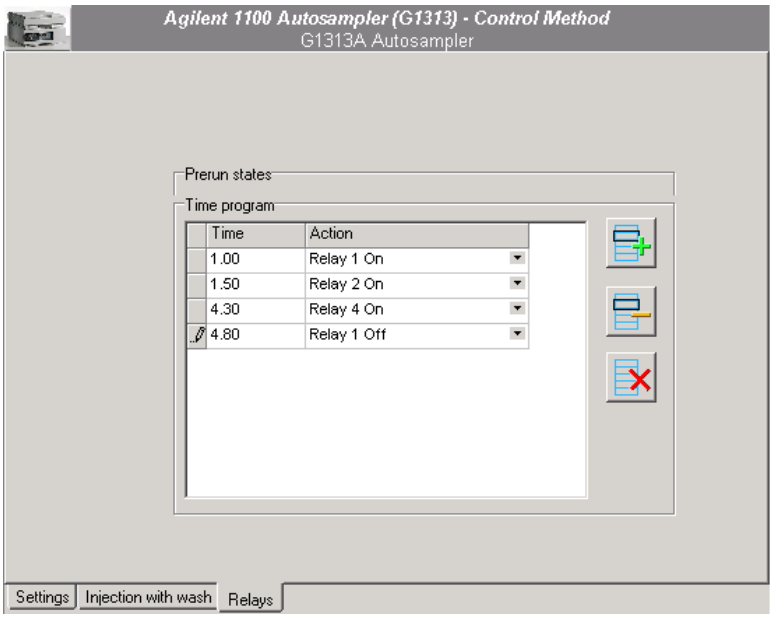
Use the scrolling list to choose the action to program. The available actions are:

- Draw from Sample
- Draw from Vial
- Draw from Seat
- Draw from Air
- Eject into Sample
- Eject into Vial
- Eject into Seat
- Eject into Air
- Mix in capillary
- Mix in air
- Wait
- Inject
- Valve Mainpass
- Valve Bypass
- Valve Mainpass with start pulse
- Valve Mainpass for a time, needle in sample vial
- Valve Mainpass for a time, needle in vial
- Valve Mainpass for a time, needle in seat
- Move Needle to uppermost position
- Move Needle to seat
- Move Needle to sample vial
- Move Needle to vial
- Move Syringe back
- Move Syringe forth
- Move Syringe back and forth
- Move Syringe home
- Move Syringe service
- Move vial to new location

Depending on the selected action, the parameters to fill in will be different.

Relays tab

If a relay board option is configured, another tab is available:



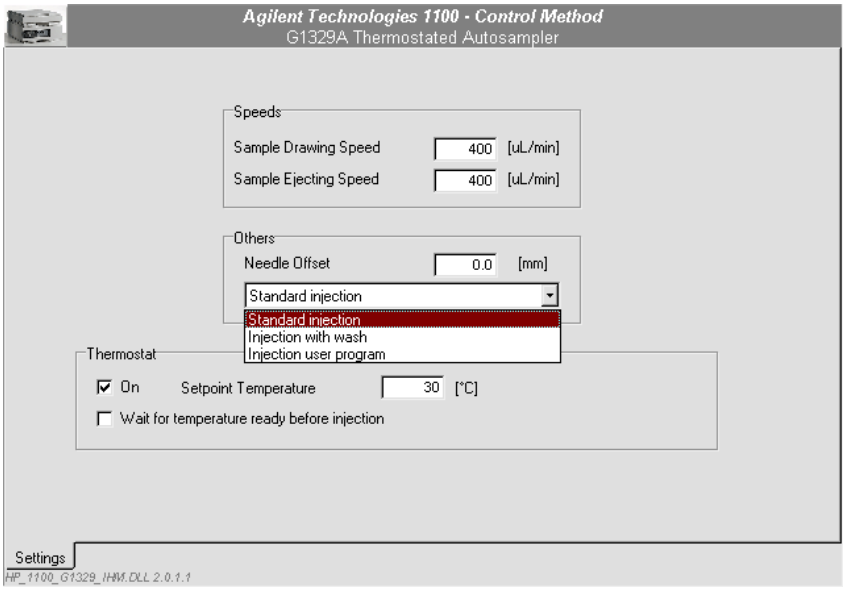
User can define the relay program.

Relay ON means the relay is closed.

Control Section for the Agilent 1260 Thermostated AutoSampler (G1329)

Click on the

button to display the Agilent Technologies 1260 Thermostated AutoSampler (G1329) control method section and to define the corresponding parameters that will be used during the chromatographic run.



Speeds Parameter Group

In the Sample Drawing Speed field, enter the sample aspiration speed value.

In the Sample Ejecting Speed field, enter the sample injection speed value.

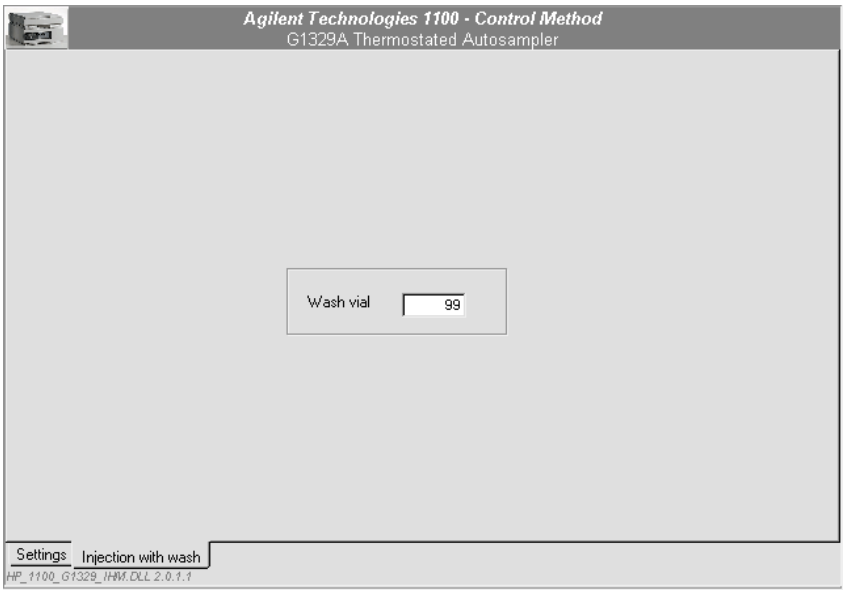
Others Parameter Group

In the Needle Offset field, enter the vertical needle offset value.

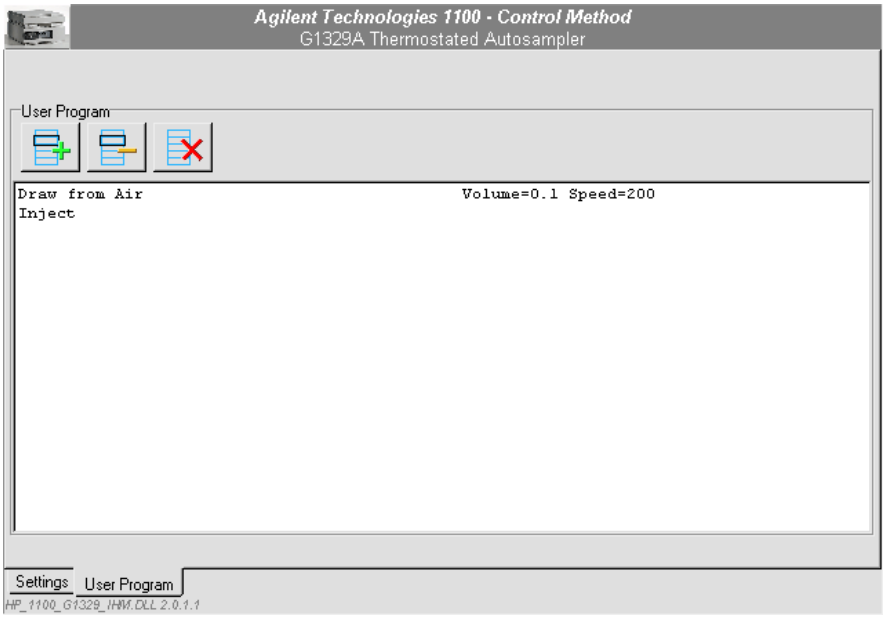
Select the injection mode in the scrolling list. Three choices are available: Standard injection, Injection with wash and Injection user program.

Standard injection: only the default screen is displayed. No other parameters are displayed.

Injection with wash: when selecting this injection mode, another tab is displayed allowing the user to define the Wash vial.



- Injection user program: when selecting this injection mode, another tab is displayed allowing the user to program different actions.



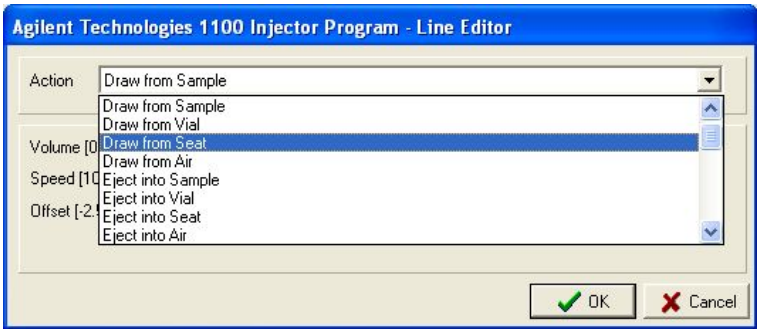
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

After a new line has been added, double-click on it to edit. A new window is displayed:



Use the scrolling list to choose the action to program. The available actions are:

Draw from Sample
Draw from Vial
Draw from Seat
Draw from Air
Eject into Sample
Eject into Vial
Eject into Seat

Eject into Air
Mix in capillary
Mix in air
Wait
Inject
Valve Mainpass
Valve Bypass
Valve Mainpass with start pulse
Valve Mainpass for a time, needle in sample vial
Valve Mainpass for a time, needle in vial
Valve Mainpass for a time, needle in seat
Move Needle to uppermost position
Move Needle to seat
Move Needle to sample vial
Move Needle to vial
Move Syringe back
Move Syringe forth
Move Syringe back and forth
Move Syringe home
Move Syringe service
Move vial to new location

Depending on the selected action, the parameters to fill in will be different.

Thermostat parameter group:

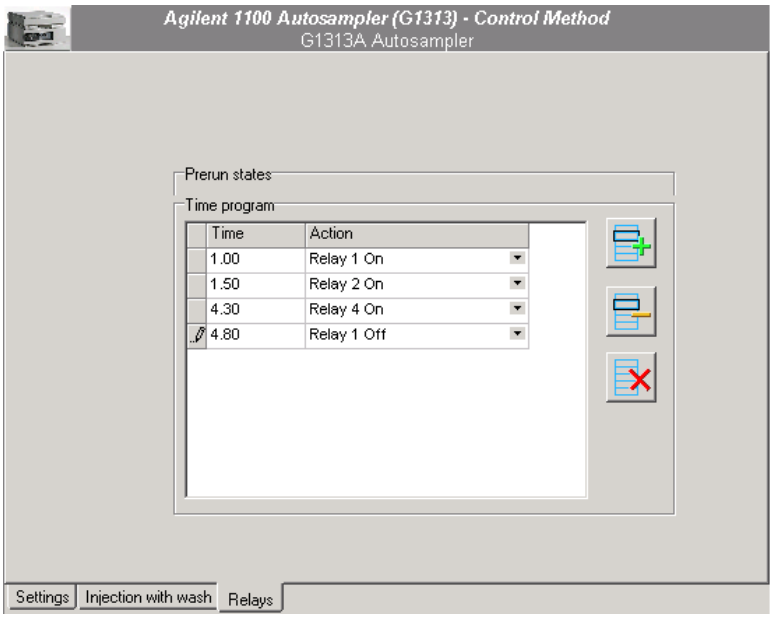
Check the On box to activate the autosampler temperature regulation.

Enter the setpoint temperature for the thermostat autosampler in the Setpoint Temperature field.

Check Wait for temperature ready before injection if necessary.

Relays tab

If a relay board option is configured, another tab is available:



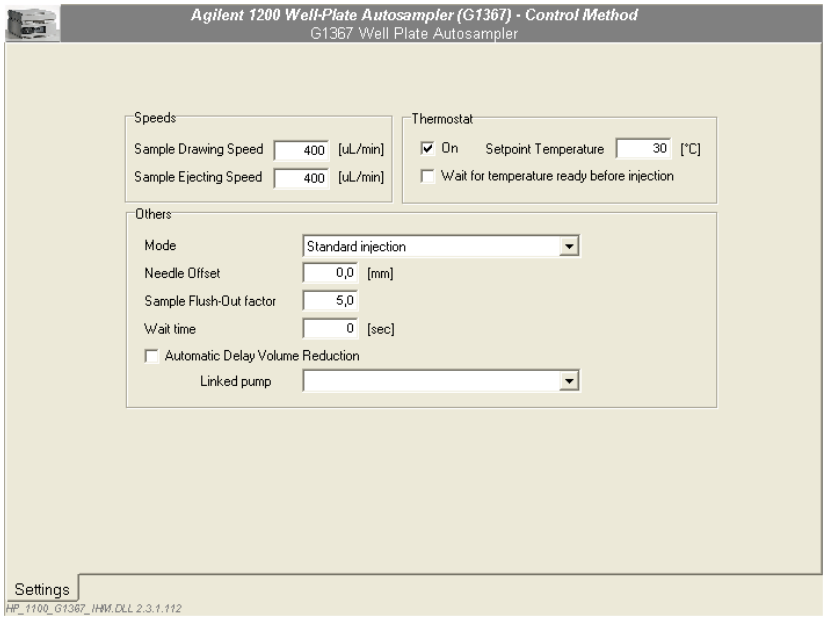
User can define the relay program.

Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Well Plate AutoSampler (G1367)

Click on the

button to display the Agilent Technologies 1260 Well Plate AutoSampler (G1367) control method section and to define the corresponding parameters that will be used during the chromatographic run.



Speeds Parameter Group

In the Sample Drawing Speed field, enter the sample aspiration speed value.

In the Sample Ejecting Speed field, enter the sample injection speed value.

Thermostat Parameter Group

Check the On box to activate the autosampler temperature regulation.

Enter the setpoint temperature for the thermostat autosampler in the Setpoint Temperature field.

Check Wait for temperature ready before injection if necessary.

Others Parameter Group

In the Needle Offset field, enter the vertical needle offset value.

In the Sample Flush-Out factor field, enter the flush out factor value that specifies the volume of mobile phase pumped through the injector after each injection.

Check Automatic Delay Volume Reduction to leave the valve in the bypass position even past analysis. Select the linked pump in the scrolling list.

In the Wait time field, enter the wait time after drawing the sample.

Select the injection mode in the scrolling list. Two choices are available: Standard injection and Injection with wash.

- Standard injection: only the default screen is displayed. No other parameters are displayed.
- Injection with wash: when selecting this injection mode, another tab is displayed allowing the user to define multiple parameters.

  Select in the drop down list the type wash. Three choices are available: Wash needle in flush port, Wash needle in wash vial, and Flush the seat.

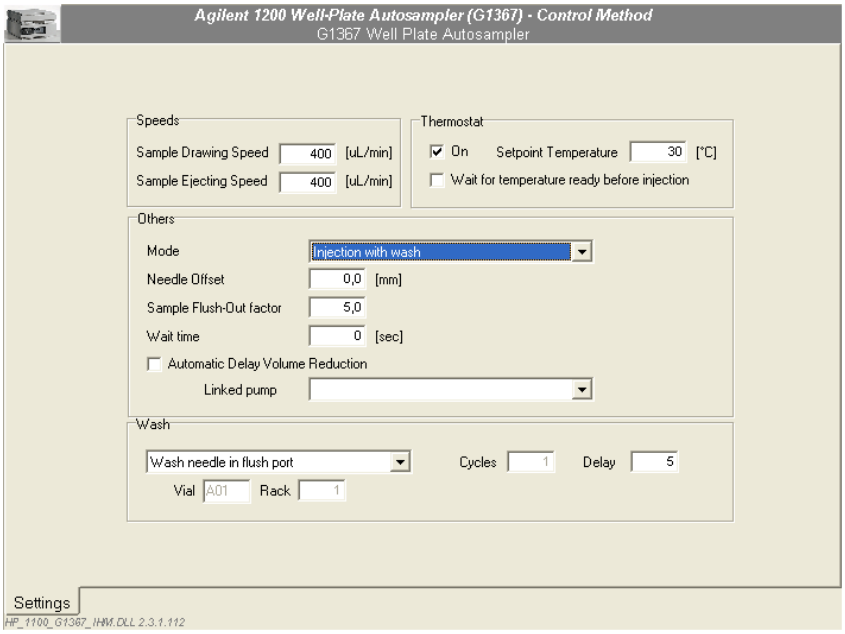
  Depending of the wash type, the following fields will be available.

  Rack: define in which rack the wash vial is located.

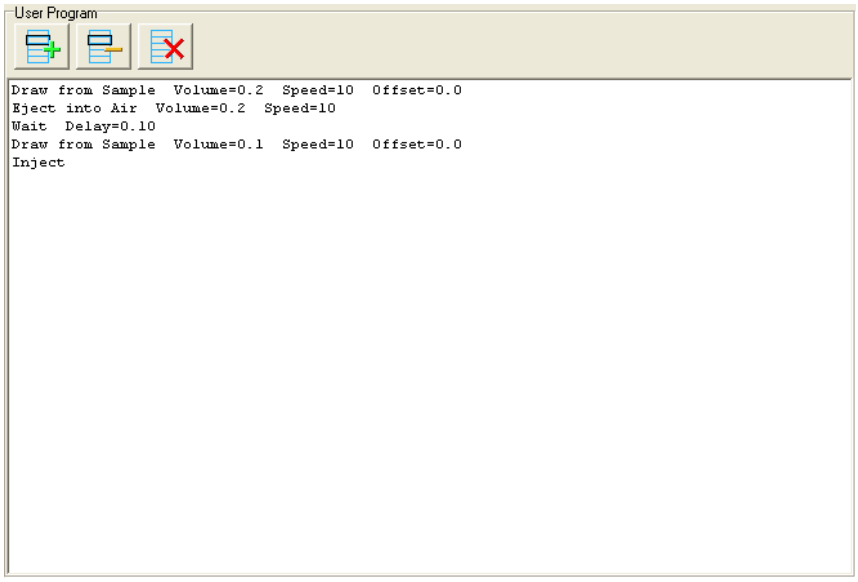
  Vial: define the location of the wash vial.

  Cycles: define the number of time the wash procedure will be done.

  Delay: define the time the needle will stay in the wash port or flush the seat.



- Injection user-program: when selecting this injection mode, another is displayed allowing you to program different actions.



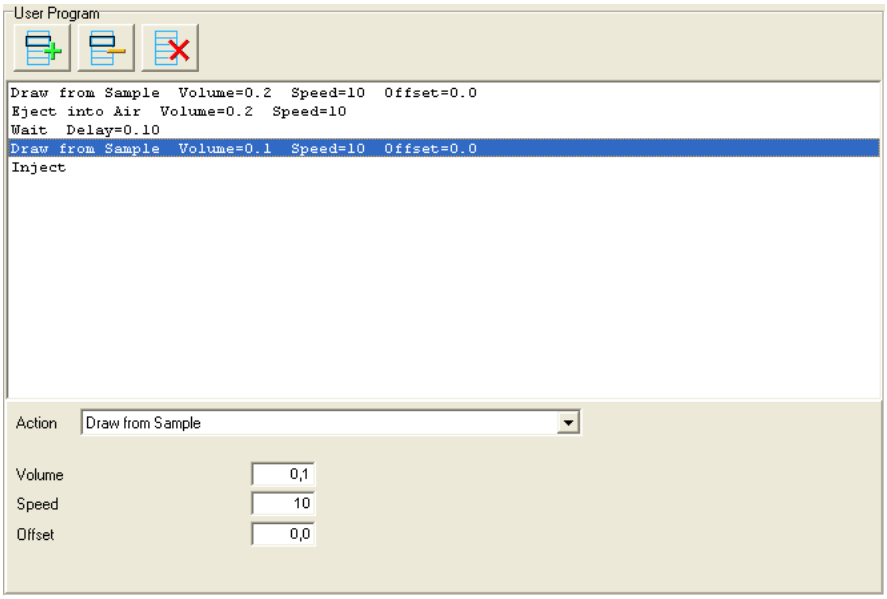
Use the following buttons to edit the table:

to add a line to the table

to delete a line in the table

to clear the entire table

After a new line has been added, double-click on it to edit. A field will be displayed:



Use the scrolling list to choose the action to program. The available actions are:

Draw from vial
Draw from seat
Draw from air
Eject into sample
Eject into sample
Eject into vial
Eject into seat
Eject into air
Mix in seat
Mix in air
Wait
Inject
Valve Mainpass
Valve Bypass
Valve Mainpass with start pulse
Valve Mainpass for a time, needle in sample vial
Valve Mainpass for a time, needle in vial
Valve Mainpass for a time, needle in seat
Move Needle to uppermost position
Move Needle to seat
Move Needle to sample vial
Move Needle to vial
Move Syringe back
Move Syringe forth
Move Syringe home

Move Syringe service
Wash needle in flush port
Wash needle in wash vial
Wash the seat
Peristaltic pump off
Peristaltic run forward
Peristaltic run backward
Peristaltic run forward for a time
Peristaltic run backward for a time

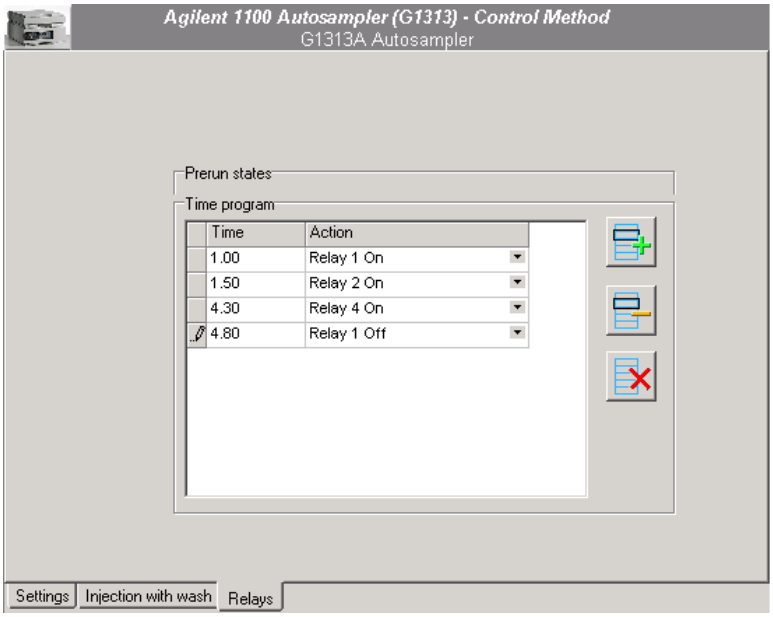
Depending on the selected action, the parameters to fill in will be different.

When an action to program is complete, click on the Apply button in order to update the table.

NOTE: When the Well Plate is selected in the system configuration in the Configuration Manager, the way to indicate the vial number is the coordinates of the well. For the third rack, with ten 2mL vials, indicate them rack 3, and vials from A01 to A10.

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

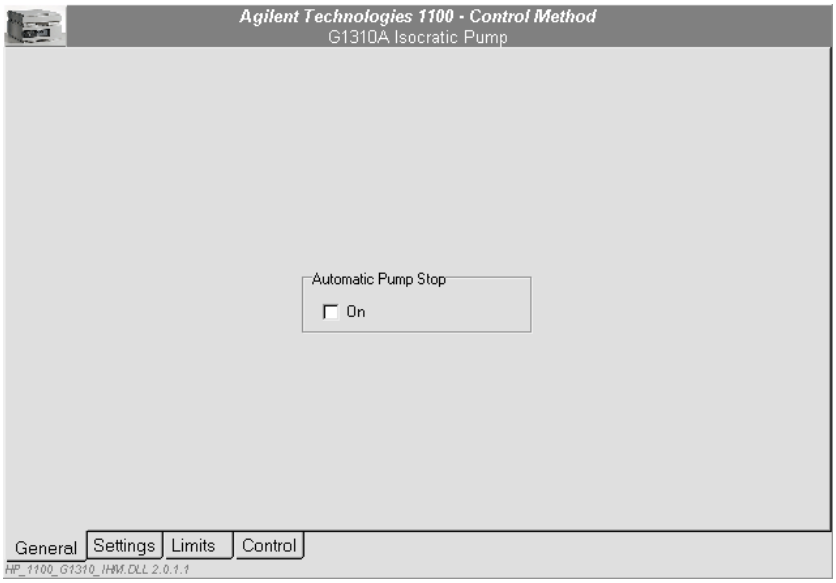
Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Isocratic Pump (G1310)

Click on the

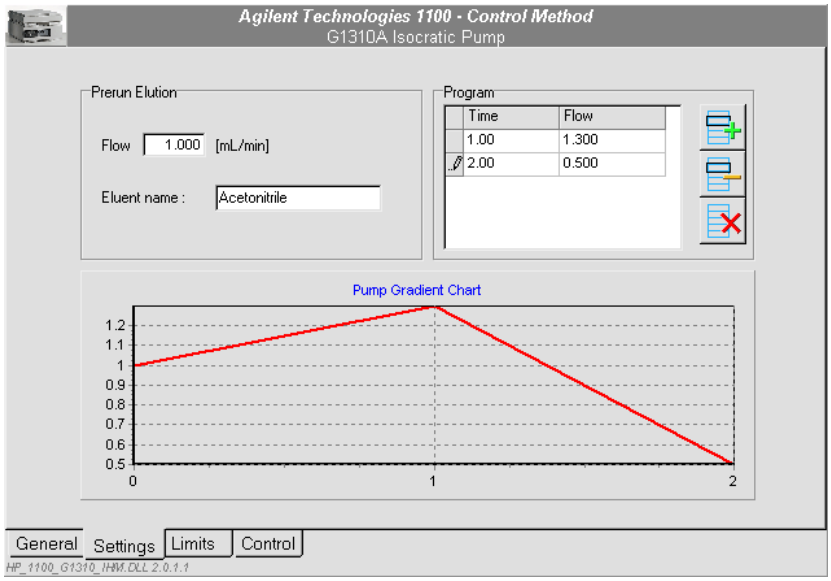
button to display the Agilent Technologies 1260Isocratic pump (G1310) control method section. It contains four sub-sections: General, Settings, Limits and Control. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

General Control



Check Automatic Pump Stop to turn off the pump at the end of a sequence.

Settings Control



Prerun Elution Parameter Group

In the Flow field, enter the total flow rate.

In the Eluent name field, enter the solvent name (optional).

Program Parameter Group

Program a flow. The time is the elapsed time since the beginning of the run. The chart represents the flow evolution.

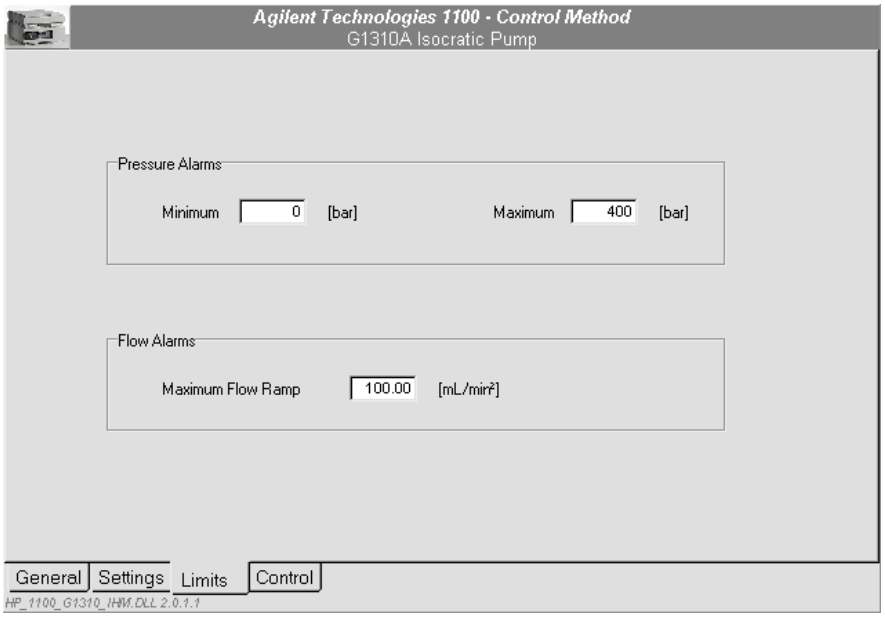
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Limits Control



Pressure Alarms Parameter Group

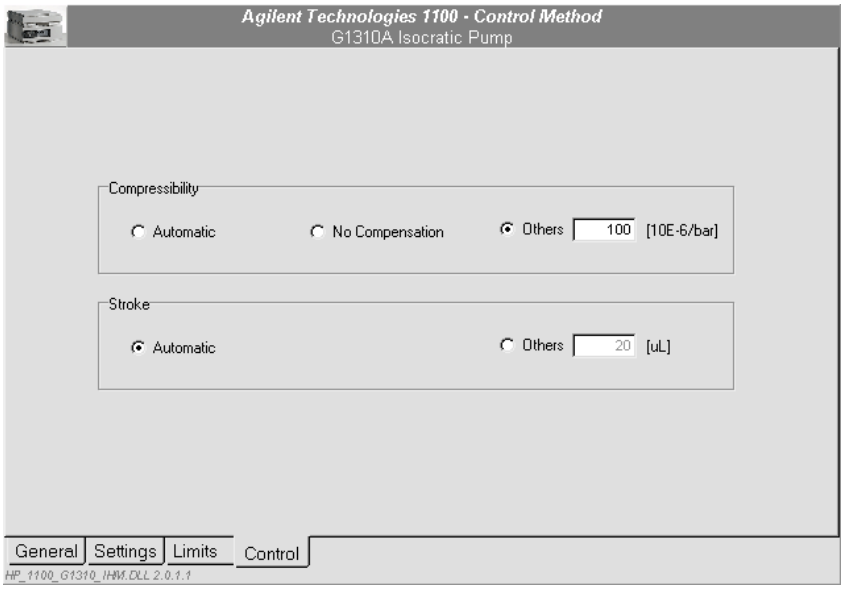
Enter the Minimum and Maximum pressure limits of the pump. Outside these limits, the pump is stopped.

For a G1310A pump, the Maximum limit is 400.0 bar. For a G1310B pump, the limit is 600.0 bar.

Flow Alarms Parameter Group

Enter the Maximum Flow Ramp of the pump. Outside this limit, the pump is stopped.

Control Control



Compressibility Parameter Group

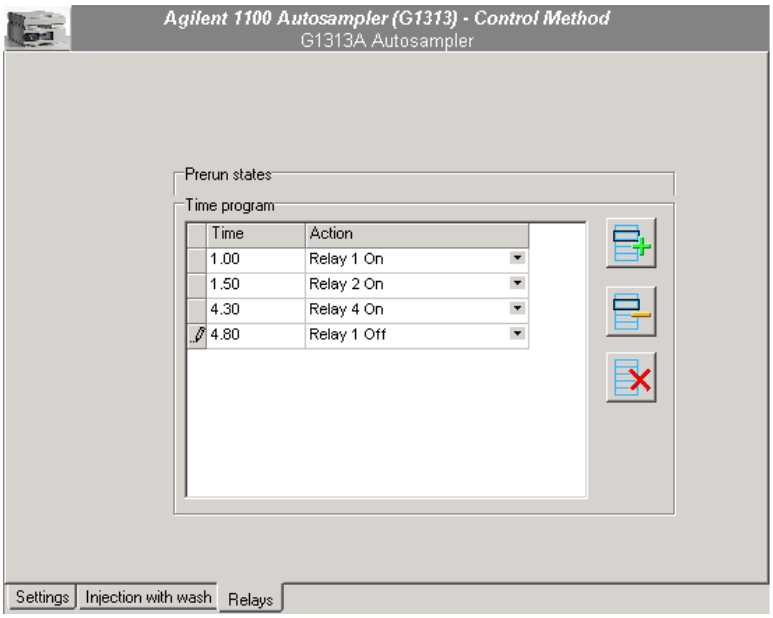
To take into account the compressibility of the solvents, select one of the available three choices: Automatic, No compensation, or Others (in this case, enter the value of the compressibility).

Stroke Parameter Group

Select the volume of the mobile phase which is moved every plunger stroke. Two choices are available: Automatic or Others (in this case, enter the volume of the mobile phase which will be moved every plunger stroke).

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Quaternary Pump (G1311)

Click on the

button to display the Agilent Technologies 1260Quaternary pump (G1311 and G5611 modules) control method section. It contains four sub-sections: General, Settings, Limits and Control. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

General Control

Miscellaneous Parameter Group

Check Automatic Pump Stop to turn off the pump at the end of a sequence.

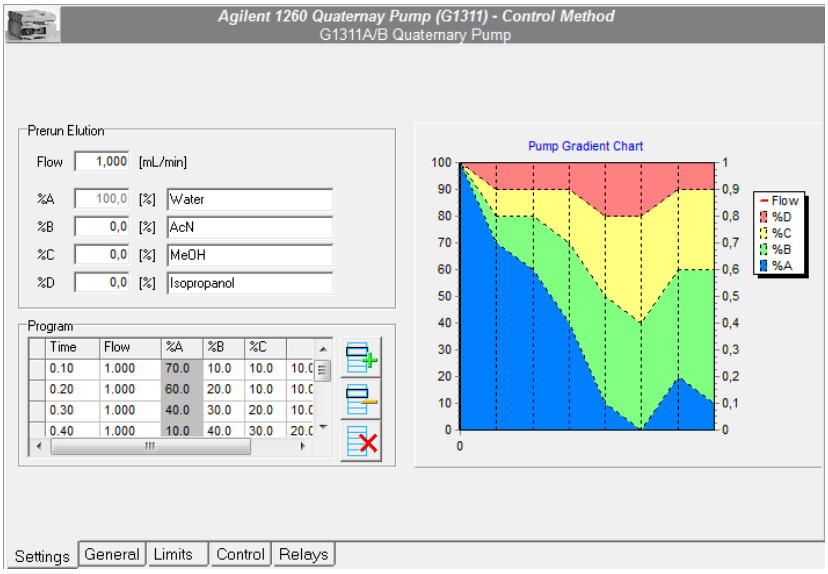
Active Seal Wash Option Parameter Group

Select Off to disable the Active Seal Wash Option.

Select Single Wash to perform a single wash. Enter the desired wash time in the Duration field.

Select Periodic to perform periodic washes. Enter the Period and On-time in the corresponding fields.

Settings Control



Prerun Elution Parameter Group

In the Flow field, enter the total flow rate.

Enter the mobile phase composition by entering the percentage of each solvent in the corresponding field.

The %A field is a read-only field. The %A value is automatically calculated according to the other solvent percentage values.

Enter the name of each solvent (optional).

Program Parameter Group

Program a flow and/or a composition gradient. Each step of the program includes time and new values for flow and/or composition. The time is the elapsed time since the beginning of the run. The Pump Gradient Chart represents the pump program.

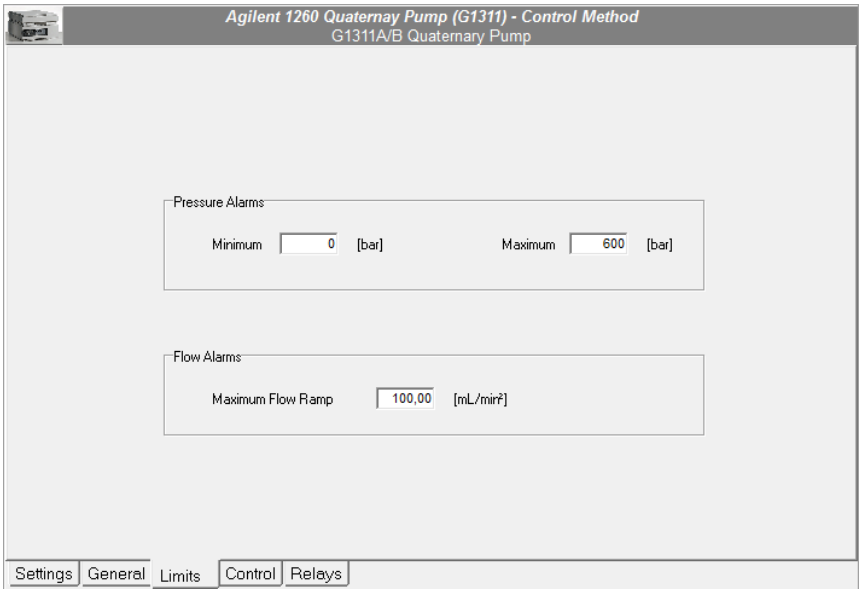
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Limits Control



Pressure Alarms Parameter Group

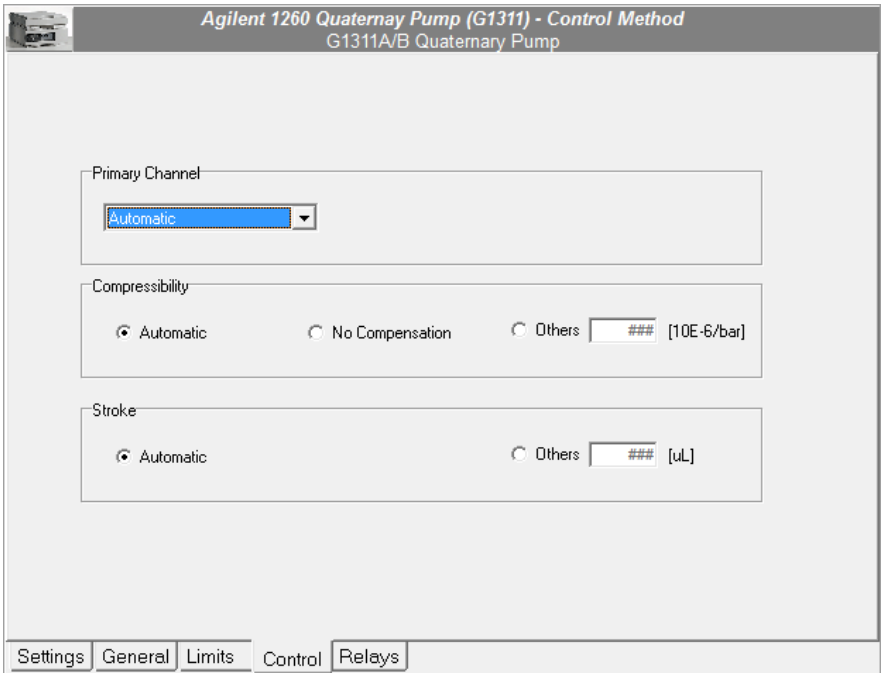
Enter the Minimum and Maximum pressure limits of the pump. Outside these limits, the pump is stopped.

For a G1311A pump, the Maximum limit is 400.0 bar. For a G1311B or G5611A pump, the limit is 600.0 bar

Flow Alarms Parameter Group

Enter the Maximum Flow Ramp of the pump. Outside this limit, the pump is stopped.

Control Control



Primary Channel Parameter Group

Select in the scrolling list the channel where the following actions will be done. The available choices are: Automatic, Channel A, Channel B, Channel C, Channel D.

Compressibility Parameter Group

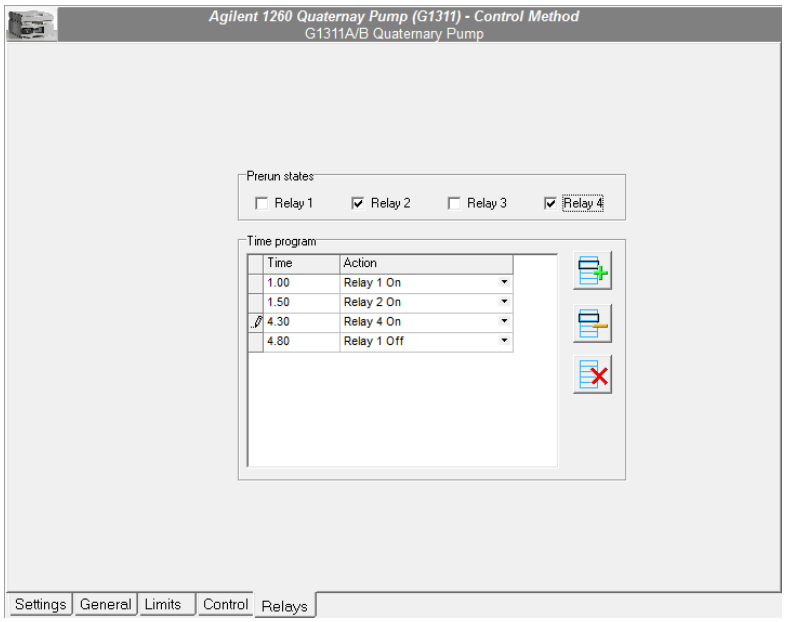
To take into account the compressibility of the solvents, select one of the three available choices: Automatic, No compensation, or Others (in this case, enter the value of the compressibility).

Stroke Parameter Group

Select the volume of the mobile phase which is moved every plunger stroke. Two choices are available: Automatic or Others (in this case, enter the volume of the mobile phase which will be moved every plunger stroke).

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

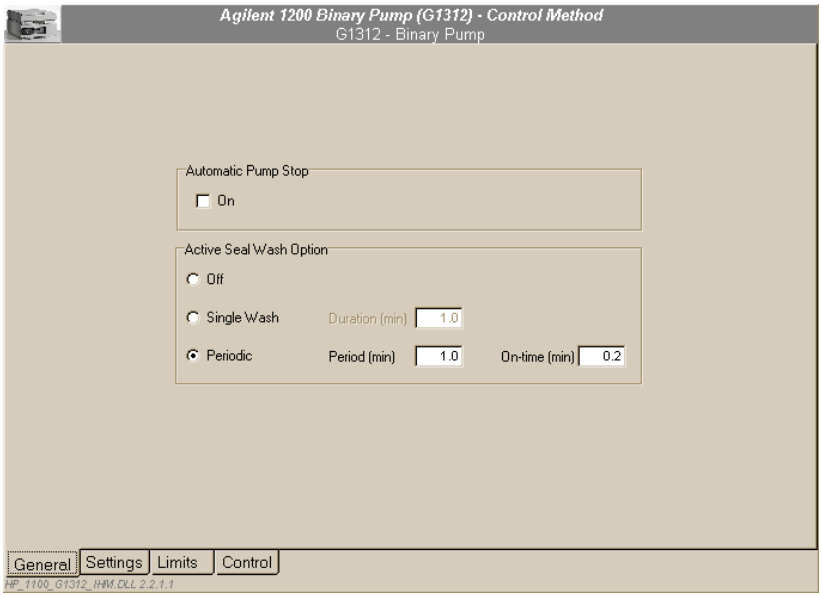
Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Binary Pump (G1312)

Click on the

button to display the Agilent Technologies 1260Binary pump (G1312) control method section. It contains four sub-sections: General, Settings, Limits and Control. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

General Control

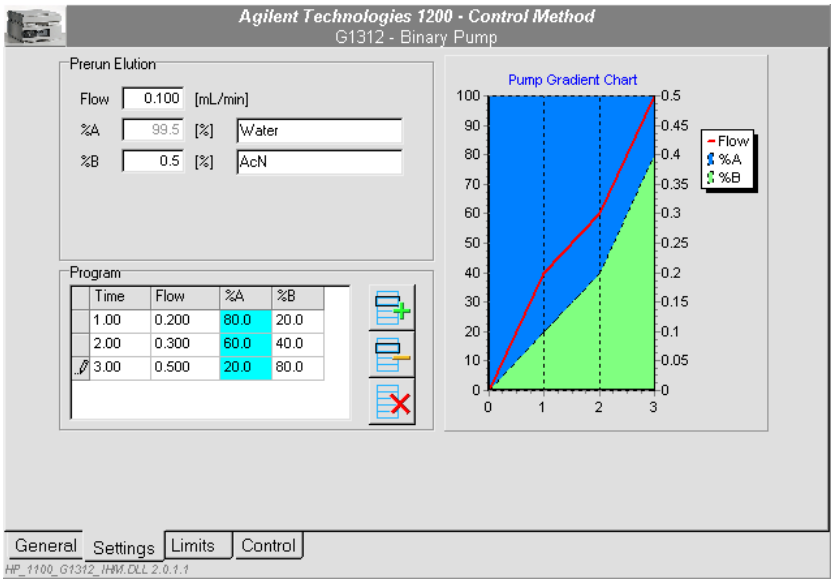


Select Off to disable the Active Seal Wash Option.

Select Single Wash to perform a single wash. Enter the desired wash time in the Duration field.

Select Periodic to perform periodic washes. Enter the Period and On-time in the corresponding fields.

Settings Control



Prerun Elution Parameter Group

In the Flow field, enter the total flow rate.

Enter the mobile phase composition by entering the percentage of the solvent B in the %B field.

The %A field is a read-only field. The %A value is automatically calculated according to the %B value.

Enter the name of each solvent (optional).

For Solvent Selection Valves A and B, choose the solvent selection channel.

Program Parameter Group

Program an elution flow and/or a composition gradient. Each step of the program includes time, flow and/or composition new values. The time is the elapsed time since the beginning of the run. The Pump Gradient Chart represents pump program.

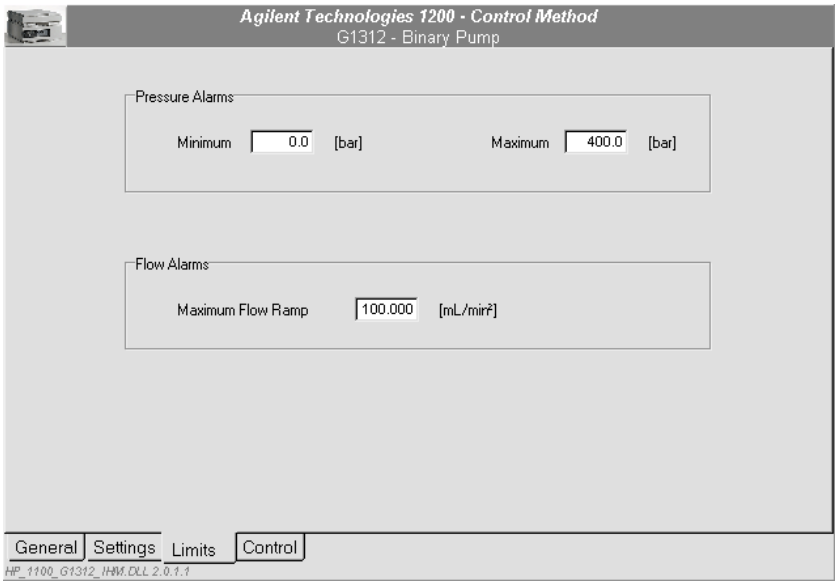
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Limits Control



Pressure Alarms Parameter Group

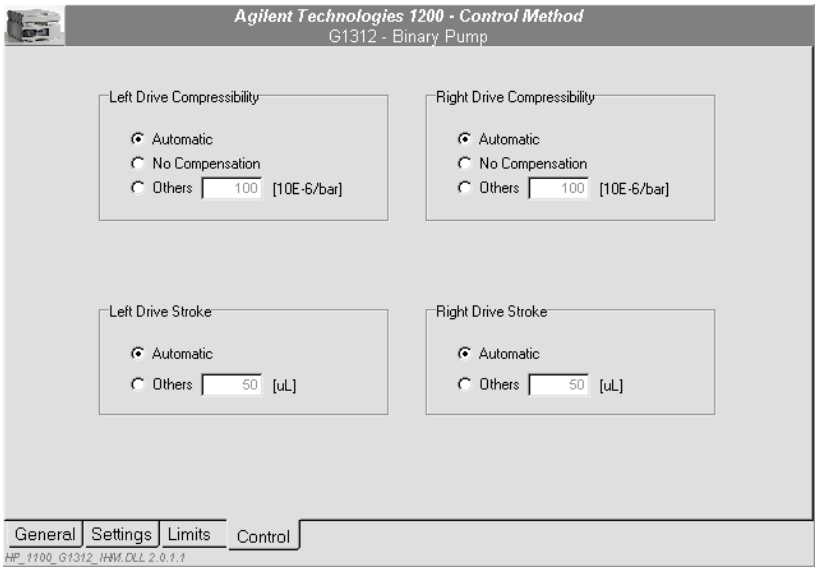
Enter the Minimum and Maximum pressure limits of the pump. Outside these limits, the pump is stopped.

For a G1312A and G1312C pumps, the Maximum limit is 400.0 bar. For a G1312B pump, the limit is 600.0 bar.

Flow Alarms Parameter Group

Enter the Maximum Flow Ramp of the pump. Outside this limit, the pump is stopped.

Control Control



Left and Right Drive Compressibility Parameter Group

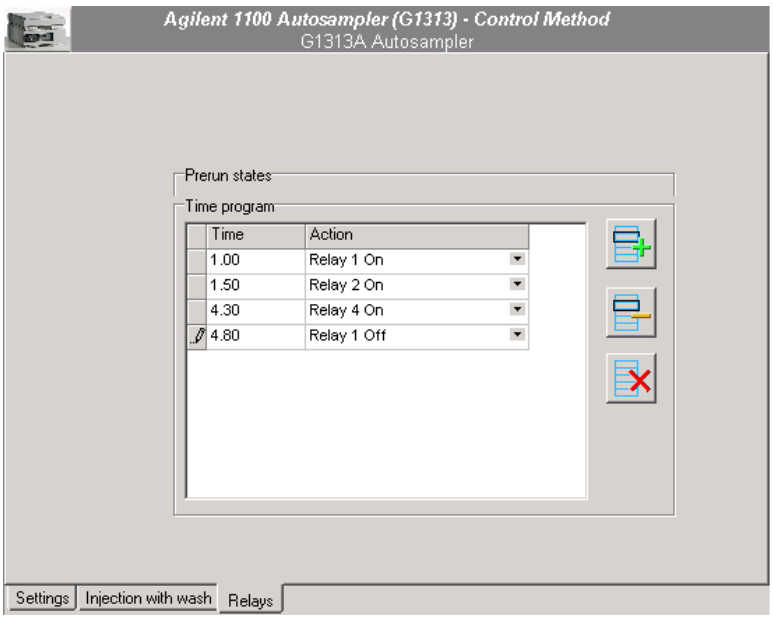
For each drive, to take into account the compressibility of the solvents, select one of the available three choices: Automatic, No compensation, or Others (in this case, enter the value of the compressibility).

Left and Right Drive Stroke Parameter Group

For each drive, select the volume of the mobile phase which is moved every plunger stroke. Two choices are available: Automatic or Others (in this case, enter the volume of the mobile phase which will be moved every plunger stroke).

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

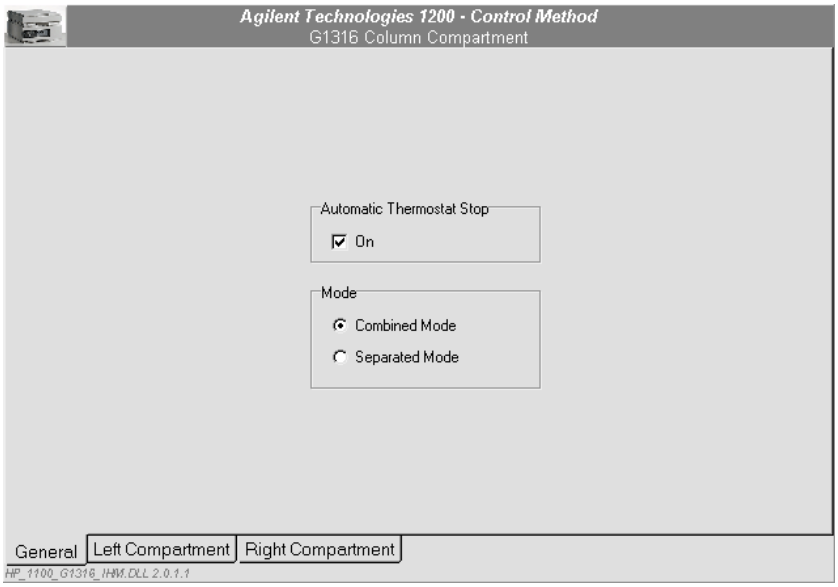
Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Column Compartment (G1316)

Click on the

button to display the Agilent Technologies 1260 Column Compartment (G1316) control method section. It contains four sub-sections: General, Left Compartment, Right Compartment and Valves. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

General Control



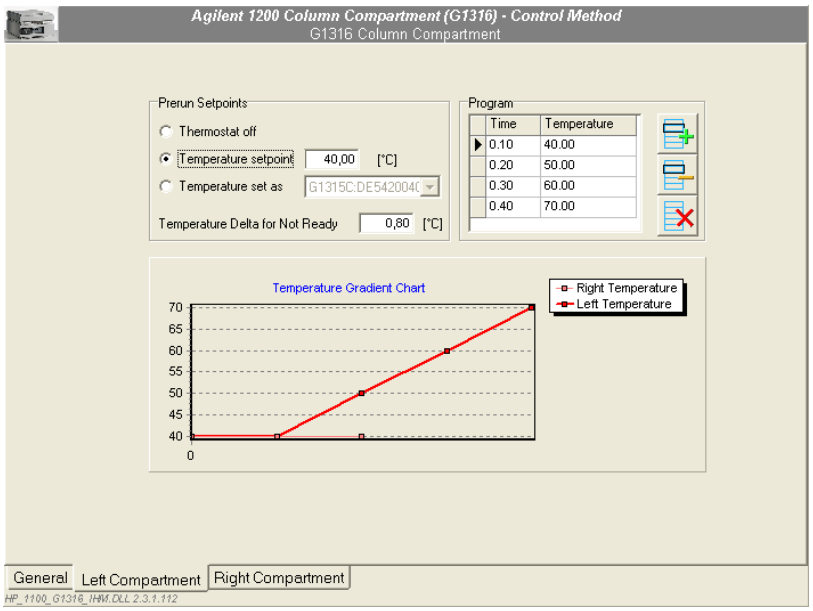
Check Automatic Thermostat Stop to turn off the thermostat at the end of the run.

Check Combined Mode to control the two column compartments in the same way. The control parameters will be entered in the Left Compartment sub-section (the Right Compartment sub-section will not be active).

Check Separated Mode to control each compartment separately. The control parameters will be entered in both Left and Right Compartment sub-sections.

Left Compartment Control

NOTE: The Left Compartment and the Right Compartment sub-sections have the same parameters. Only the Left Compartment sub-section parameters will be explained.



Left Compartment Prerun Setpoints Parameter Group

Check the On box to activate the column compartment temperature regulation.

Enter the setpoint temperature in the Temperature field in order to set the temperature and a gradient in the column compartment

Check Temperature as then select a detector, in order to set the same temperature in the column compartment then the detector cell temperature.

Enter the Temperature Delta for Not Ready in the corresponding field. Set 0 in order to bypass the wait for ready stage.

Left Compartment Program Parameter Group

Program a temperature. The time is the elapsed time since the beginning of the run. The chart represents the temperature evolution.

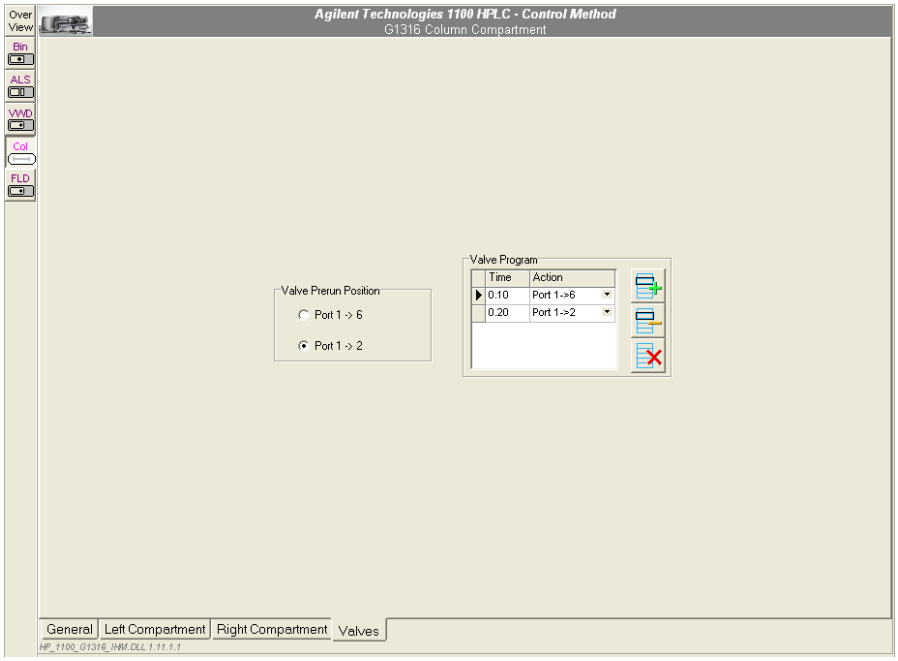
Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Valves Control



Valve Prerun Position Parameter Group

Select the position of the valve before the run begins. The available choices are: Port 1>6 and Port 1>2

Valve Program Parameter Group

Program valve position changes during the run. The time is the elapsed time since the beginning of the run.

Use the following buttons to edit the table:

to add a line to the table.

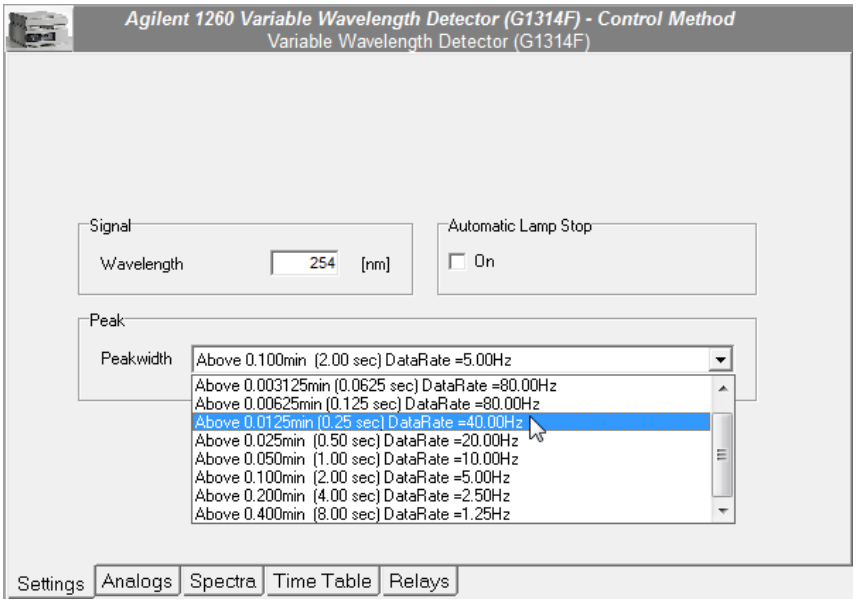
to delete a line in the table.

to clear the entire table.

Control Section for the Agilent LC 1260 Variable Wavelength Detector (G1314)

Click on the button to display the Agilent Technologies 1260Variable Wavelength Detector (G1314) control method section. It contains four sub-sections: Settings, Analogs, Spectra and Time table. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Settings Control



Signal Parameter Group

In the Wavelength field, enter the value of the initial Wavelength.

Automatic Lamp Stop Parameter Group

Check Automatic Lamp Stop to stop automatically the detector lamp at the end of the run.

Peak Parameter Group

Select the Peakwidth value in the scrolling list. This parameter influences the peak detection. A response time and a data rate are associated with each peakwidth value. The available values are:

For the G1314 A/B (Agilent Technologies 1260 LC):

Below 0.0063min (0.125 sec) DataRate =13.74Hz

Above 0.0063min (0.125 sec) DataRate =13.74Hz

Above 0.0125min (0.25 sec) DataRate =13.74Hz

Above 0.025min (0.50 sec) DataRate =13.74Hz

Above 0.050min (1.00 sec) DataRate =6.87Hz

Above 0.100min (2.00 sec) DataRate =3.43Hz

Above 0.200min (4.00 sec) DataRate =1.72Hz

Above 0.400min (8.00 sec) DataRate =0.86Hz

For the G1314 C (Agilent Technologies 1260 LC):

Below 0.0016min (0.032 sec) DataRate =54.95Hz

Above 0.0016min (0.032 sec) DataRate =24.47Hz

Above 0.0032min (0.063 sec) DataRate =13.74Hz

Above 0.0063min (0.125 sec) DataRate =13.74Hz

Above 0.0125min (0.25 sec) DataRate =13.74Hz

Above 0.025min (0.50 sec) DataRate =13.74Hz

Above 0.050min (1.00 sec) DataRate =6.87Hz

Above 0.100min (2.00 sec) DataRate =3.43Hz

Above 0.200min (4.00 sec) DataRate =1.72Hz

Above 0.400min (8.00 sec) DataRate =0.86Hz

For the G1314 D (Agilent Technologies 1200 LC):

Below 0.0063min (0.032 sec) DataRate =20.00Hz

Above 0.0063min (0.125 sec) DataRate =20.00Hz

Above 0.0125min (0.25 sec) DataRate =20.00Hz

Above 0.025min (0.50 sec) DataRate =20.00Hz

Above 0.050min (1.00 sec) DataRate =10.00Hz

Above 0.100min (2.00 sec) DataRate =5.00Hz

Above 0.200min (4.00 sec) DataRate =2.50Hz

Above 0.400min (8.00 sec) DataRate =1.25Hz

For the G1314 E (Agilent Technologies 1200 LC):

Below 0.0015625min (0.03125 sec) DataRate =160.00Hz

Above 0.0015625min (0.03125 sec) DataRate =160.00Hz

Above 0.003125min (0.0625 sec) DataRate =160.00Hz

Above 0.00625min (0.125 sec) DataRate =80.00Hz

Above 0.0125min (0.25 sec) DataRate =40.00Hz

Above 0.025min (0.50 sec) DataRate =20.00Hz

Above 0.050min (1.00 sec) DataRate =10.00Hz

Above 0.100min (2.00 sec) DataRate =5.00Hz

Above 0.200min (4.00 sec) DataRate =2.50Hz

Above 0.400min (8.00 sec) DataRate =1.25Hz

For the G1314 F (Agilent 1260 Infinity HPLC)

Below 0.003125min (0.0625 sec) DataRate =80.00Hz

Above 0.003125min (0.0625 sec) DataRate =80.00Hz

Above 0.00625min (0.125 sec) DataRate =80.00Hz

Above 0.0125min (0.25 sec) DataRate =40.00Hz

Above 0.025min (0.50 sec) DataRate =20.00Hz

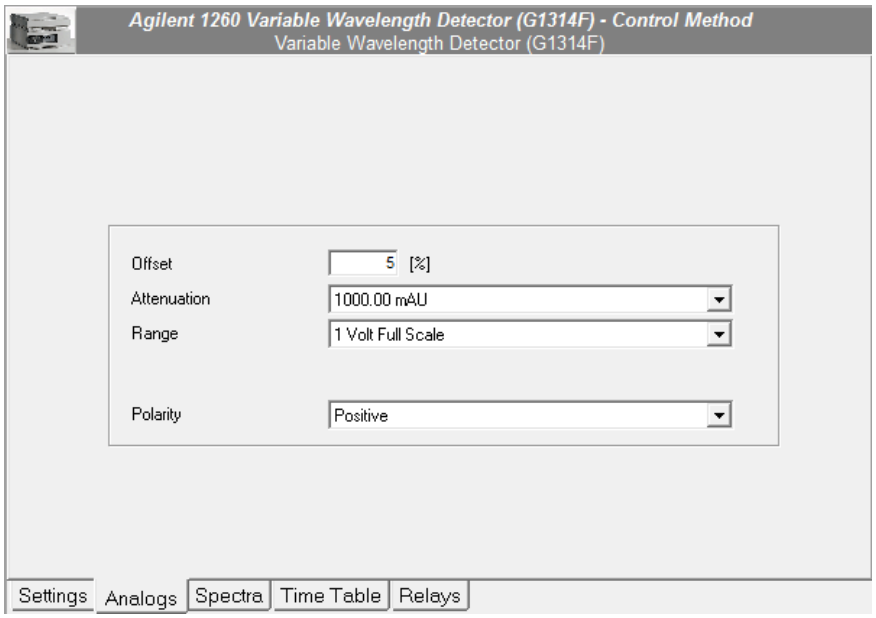
Above 0.050min (1.00 sec) DataRate =10.00Hz

Above 0.100min (2.00 sec) DataRate =5.00Hz

Above 0.200min (4.00 sec) DataRate =2.50Hz

Above 0.400min (8.00 sec) DataRate =1.25Hz

Analogs Control



In the Offset field, enter the offset value to adjust the baseline.

In the Attenuation scrolling list, enter the attenuation value. The available values are:

0.97 mAU full range, 1.95 mAU, 3.90 mAU, 7.81 mAU, 15.62 mAU, 31.25 mAU, 62.50 mAU, 125 mAU, 250 mAU, 500 mAU, 1000 mAU, 2000 mAU and 4000 mAU.

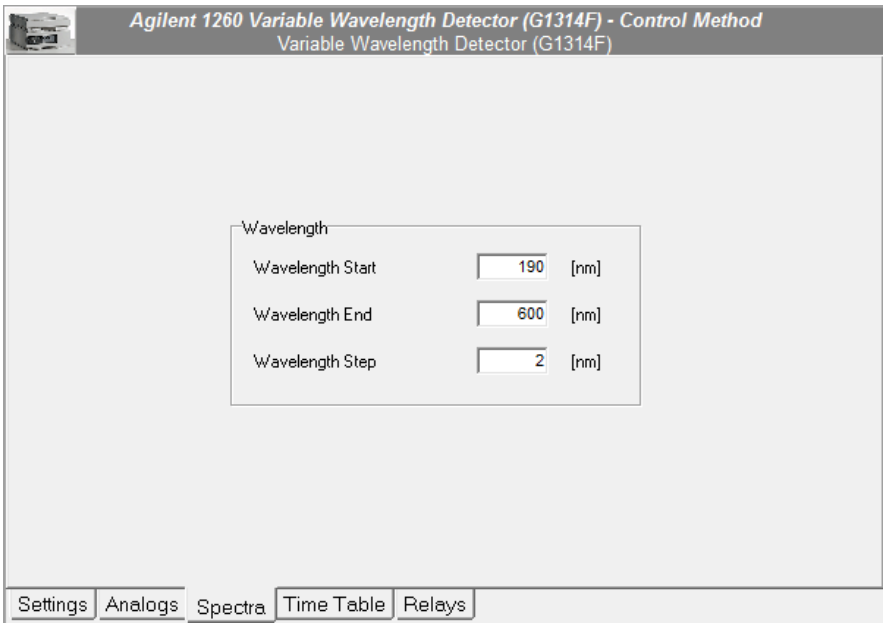
In the Range scrolling list, enter the output voltage range value. The available values are: 0.1 Volt Full Scale and 1Volt Full Scale.

In the Source scrolling list, enter the collected signal type. The available values are: Absorbance Units AU, Sample AU without Reference, Reference AU without Sample, Test Chromatogram, Unfiltered and not logarithm Sample, Unfiltered and not logarithm Reference, Analog Output Test Function, Sample Diode Current, Reference Diode Current, Lamp Anode Voltage, Lamp Anode

Current, Lamp Heater Voltage, Lamp Heater Current, Grating Motor Step, Filter Motor Step, Board Temperature and PTC current.

In the Polarity scrolling list, enter the detector polarity. The available values are: Positive and Negative.

Spectra Control



Wavelength Parameter Group

In the Wavelength Start field, enter the minimum spectra wavelength.

In the Wavelength End field, enter the maximum spectra wavelength.

In the Wavelength Step field, enter the wavelength step.

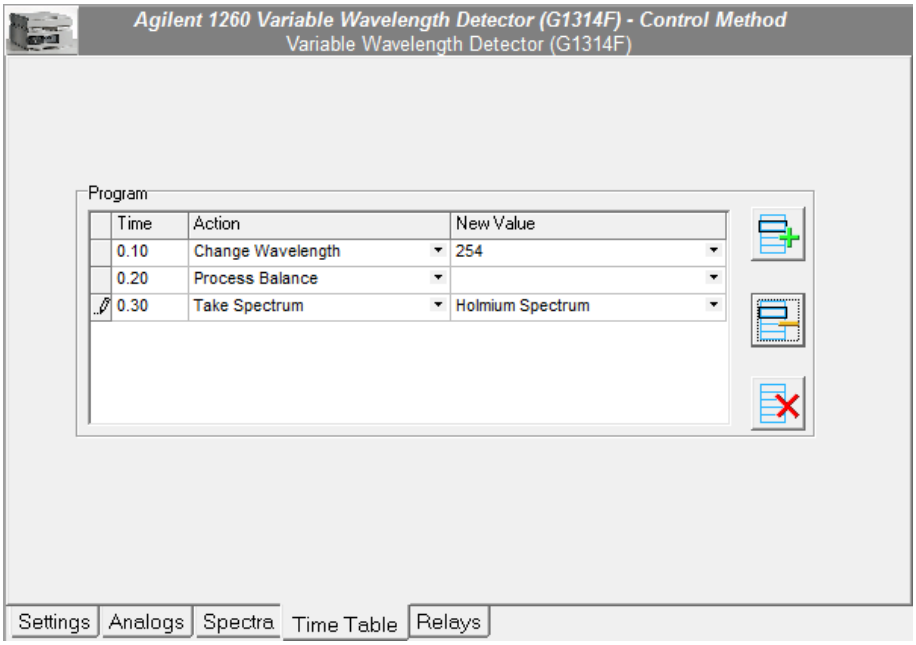
Peak Detector Parameter Group (only for G1314 A/B, and G1314 C)

In the Peak Detector Threshold field, enter the peak detector threshold value.

In the Peak Detector Peakwidth scrolling list, select the peak detector peakwidth value. A response time is associated with each peakwidth values. The available values are:

<0.005 min (RiseTime<0.12 sec)
>0.005 min (RiseTime>0.12 sec)
>0.010 min (RiseTime>0.25 sec)
>0.025 min (RiseTime>0.5 sec)
>0.05 min (RiseTime>1 sec)
>0.1 min (RiseTime>2 sec)
>0.2 min (RiseTime>4 sec)
>0.4 min (RiseTime>8 sec)

Time Table Control



Program Parameter Group

Program detector changes during the run. In the Action scrolling list, select Change Wavelength, or Change PeakWidth (only for the G1314A/B and G1314C).). It is also possible to launch an autozero, (Process Balance function) or collect spectra (Normal spectrum, Blank, Unknown and Holmium of the Take Spectrum function).

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

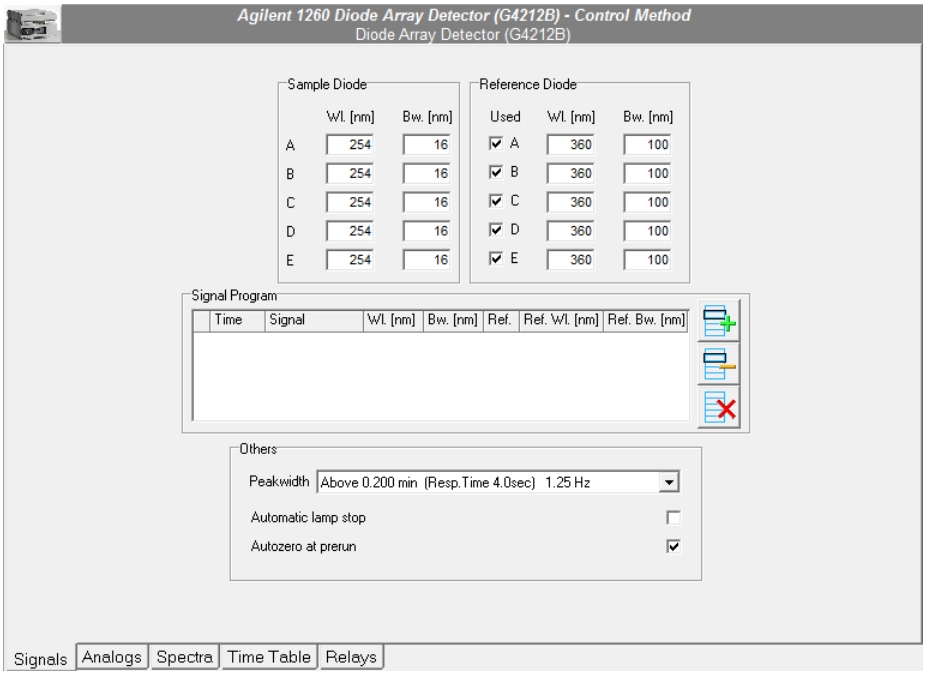
to clear the entire table.

Control Section for the Agilent LC 1260 Diode Array Detector (G1315), the Agilent LC 1260 Multiple Wavelength Detector (G1365), and the Agilent 1260 Infinity HPLC Diode Array Detector (G4212B)

Click on the

button to display the Agilent Technologies 1260LC Diode Array Detector (G1315 or G4212B) or the Multiple Wavelength Detector (G1365) control method section. It contains four sub-sections: Signals, Analogs, Spectra (only for the G1315 and the G4212B) and Time table. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Signals Control



Sample Diode Parameter Group

Define the center wavelength in the Wl field and the bandwidth in the Bw field. The signal values contained within the bandwidth are bunched and give one value for the center wavelength.

Reference Diode Parameter Group

The use of a reference wavelength avoids baseline drift due to refractive index changes.

If a reference wavelength is defined, the measured signal value is the difference between absorbance at the sample wavelength and absorbance at the reference wavelength.

Define the center wavelength in the Wl field and the bandwidth in the Bw field. The signal values contained within the bandwidth are bunched and give one value for the center wavelength.

NOTE: For more details about the reference wavelength settings, refer to your Agilent Technologies 1260Diode Array Detector technical documentation.

Signal Program Parameter Group

Program changes the wavelength and/or the bandwidth for each signal and/or its reference during runs.

Use the following buttons to edit the table:

to add a line to the table.

to delete a line in the table.

to clear the entire table.

Others Parameter Group

Check Automatic Lamp Stop to stop automatically the detector lamp at the end of the run.

Check Auto zero at prerun to perform automatically an autozero during the prerun step of the acquisition.

Select the Peakwidth value in the scrolling list. This parameter influences the peak detection. A response time and a data rate are associated with each peakwidth value. The available values are:

For the G1315C, the G1365C and the G4212B:

Below 0.0025 min (Resp. Time 0.025 sec) 80 Hz

Above 0.0025 min (Resp. Time 0.05 sec) 80 Hz

Above 0.005 min (Resp. Time 0.1 sec) 40 Hz

Above 0.01 min (Resp. Time 0.2 sec) 20 Hz

Above 0.02 min (Resp. Time 0.5 sec) 10 Hz

Above 0.05 min (Resp. Time 1.0 sec) 5 Hz

Above 0.10 min (Resp. Time 2.0 sec) 2.5 Hz

Above 0.20 min (Resp. Time 4.0 sec) 1.25 Hz

Above 0.40 min (Resp. Time 8.0 sec) 0.62 Hz

Above 0.850 min (Resp. Time 16.0 sec) 0.31 Hz

For the G1315 A/B/D and the G1365A/B/D:

Below 0.005 min (Resp. Time 0.1 sec) 20 Hz

Above 0.01 min (Resp. Time 0.2 sec) 20 Hz

Above 0.02 min (Resp. Time 0.5 sec) 10 Hz

Above 0.05 min (Resp. Time 1.0 sec) 5 Hz

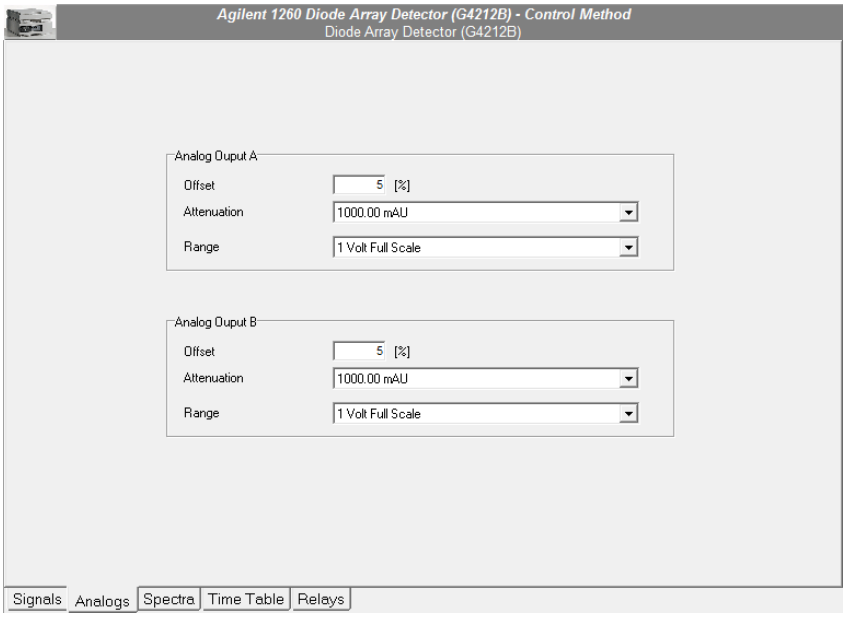
Above 0.10 min (Resp. Time 2.0 sec) 2.5 Hz

Above 0.20 min (Resp. Time 4.0 sec) 1.25 Hz

Above 0.40 min (Resp. Time 8.0 sec) 0.62 Hz

Above 0.850 min (Resp. Time 16.0 sec) 0.31 Hz

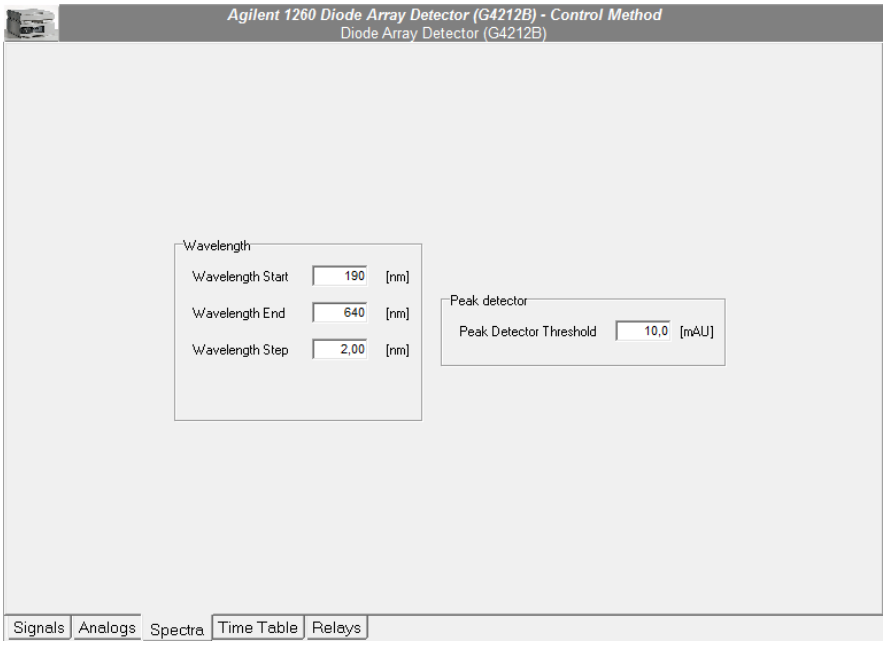
Analogs Control



This detector has two analog outputs. For each one:

- In the Offset field, enter the offset value to adjust the baseline.
- In the Attenuation scrolling list, enter the attenuation value. The available values are: 0.97 mAU full range, 1.95 mAU, 3.90 mAU, 7.81 mAU, 15.62 mAU, 31.25 mAU, 62.50 mAU, 125 mAU, 250 mAU, 500 mAU, 1000 mAU and 2000 mAU.
- In the Range scrolling list, enter the output voltage range value. The available values are: 0.1 Volt Full Scale and 1 Volt Full scale.

Spectra Control [only for the Agilent LC 1260 Diode Array Detector (G1315 and G4212B)]



Wavelength Parameter Group

In the Wavelength Start field, enter the minimum spectra wavelength.

In the Wavelength End field, enter the maximum spectra wavelength.

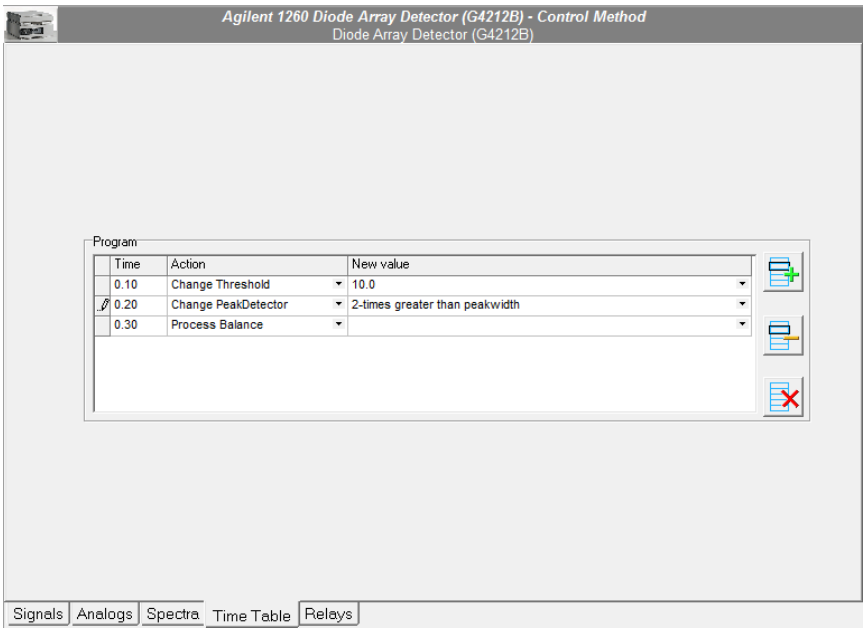
In the Wavelength Step field, enter the wavelength step.

In the Wavelength Slit scrolling list, select the wavelength slit. The available choices are: 1, 2, 4, 8 and 16 nm. This field is not available for the Agilent 1260 Infinity HPLC Diode Array Detector G4212B.

Peak Detector Parameter Group

In the Peak Detector Threshold field, enter the peak detector threshold value.

Time Table Control



Program Parameter Group

Program detector changes during the run. In the action scrolling list, select Change PeakDetector and/or Change Threshold and enter the corresponding time and new value. It is also possible to launch an autozero (Process Balance function)

Use the following buttons to edit the table:

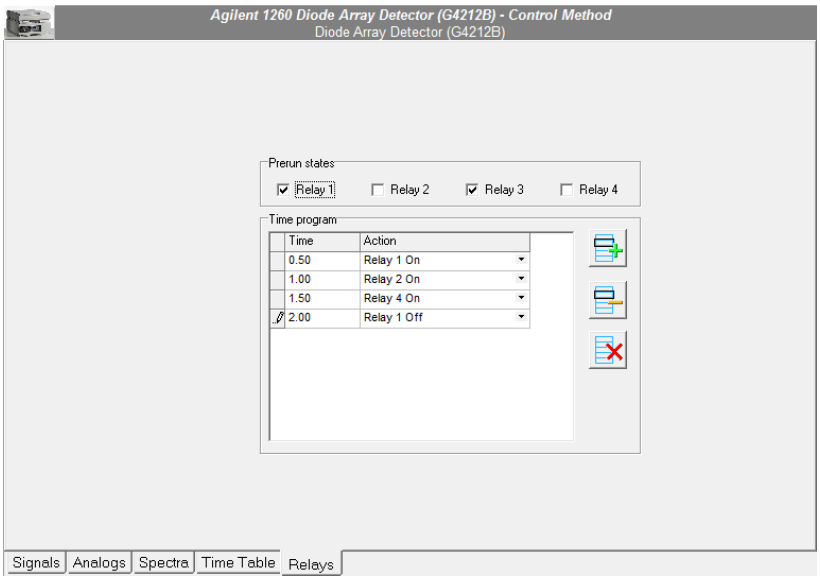
to add a line to the table.

to delete a line in the table.

to clear the entire table.

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

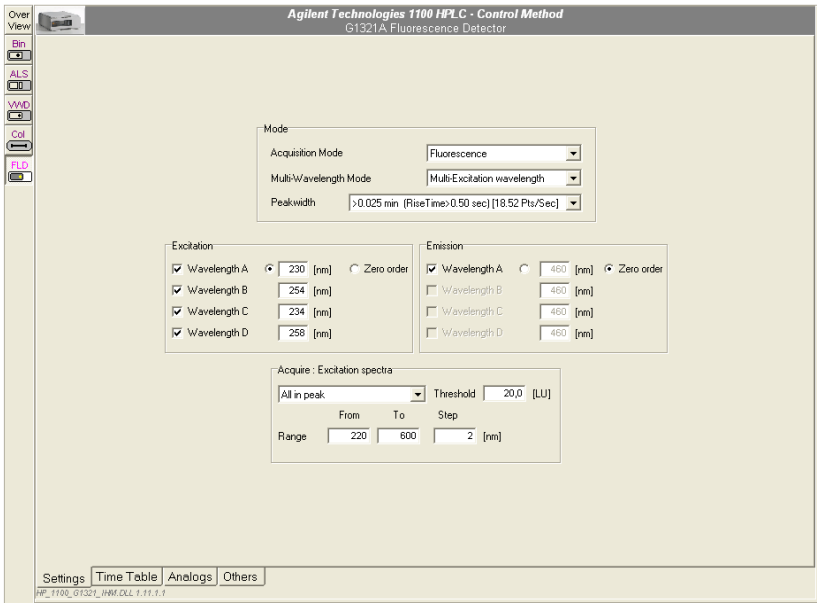
Relay ON means the relay is closed.

Control Section for the Agilent LC 1260 Fluorescence Detector (G1321)

Click on the

button to display the Agilent Technologies 1260 Fluorescence Detector (G1321) control method section. It contains five sub-sections: Settings, Analogs, Time table, Phosphorescence and Others. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Settings Control



Mode Parameter Group

Choose the Acquisition Mode. (Fluorescence, Phosphorescence, or Chemo-luminescence).

To work in emission or excitation Multi-wavelength mode, select the corresponding mode in the scrolling list. When selecting the excitation multi-wavelength mode, the wavelengths from B to D in the emission part are not accessible and vice versa.

Select in the Peakdwidth scrolling list, the peakdwidth of the detector influencing the peak detection. A response time and a data rate are associated to each peakwidth values.

Excitation Parameter Group

Check Wavelength A to Wavelength D to activate the corresponding wavelengths in multi--wavelength mode. Enter their values in the corresponding fields.

Check Zero Order to work at zero order.

Emission Parameter Group

Check Wavelength A to Wavelength D to activate the corresponding wavelengths in multi--wavelength mode. Enter their values in the corresponding fields.

Check Zero Order to work at zero order.

Acquire Spectra Parameter Group

Using the scrolling list, select the spectral Acquisition Mode.

None: no spectra are stored.

Apex: only the top of peak spectrum is stored.

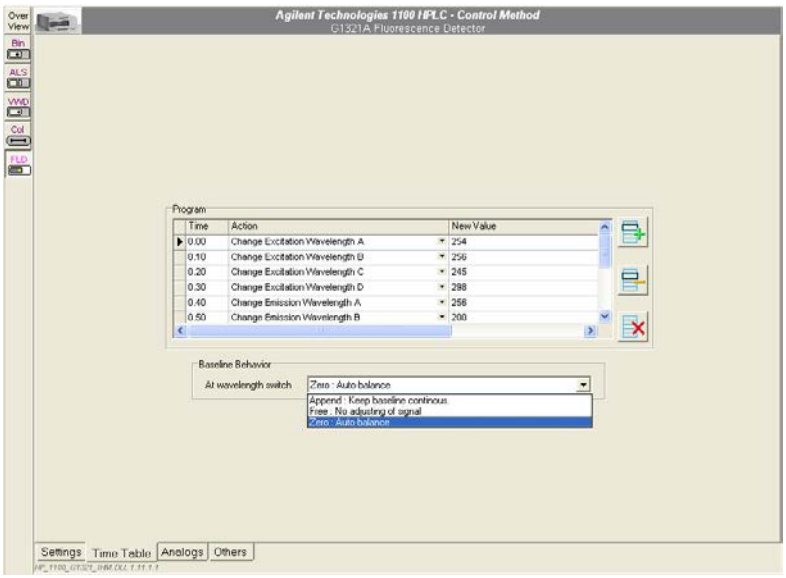
All in peak: all spectra between the beginning and the end of a peak are stored.

All: all spectra are stored during the run.

In the fields defining the Range, enter the minimum and maximum wavelength of the spectrum. Enter the wavelength Step in the corresponding field. A small wavelength step will enhance the spectrum resolution.

Enter the value of the Threshold in the corresponding field.

Time Table Control



Program Parameter Group

Program detector changes during the run. Change the excitation or emission wavelength, the peakdetector and/or the threshold values.

Use the following buttons to edit the table:

to add a line to the table.

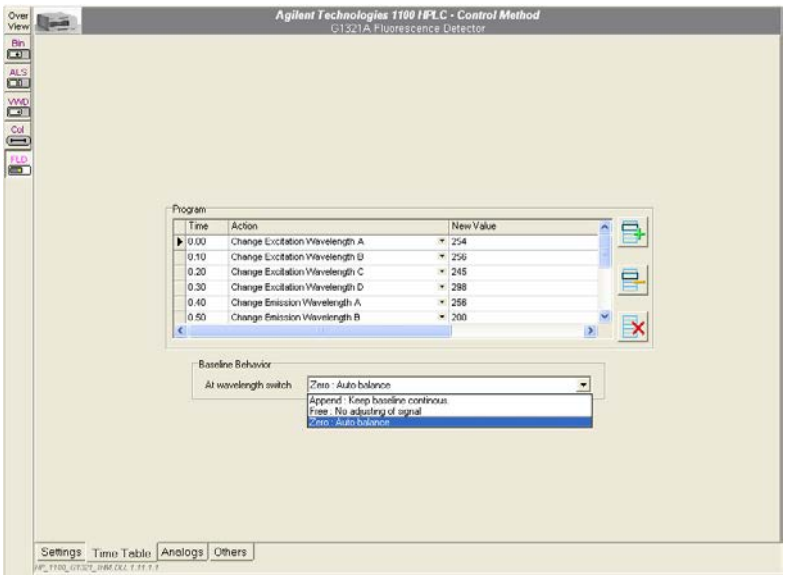
to delete a line in the table.

to clear the entire table.

Baseline Behavior Parameter Group

Select in the scrolling list the type of Baseline Behavior. Three choices are available: Append, Zero and Free.

Analogs Control



Analog Parameter Group

This detector has two analog outputs. For each one:

In the Offset field, enter the offset value to adjust the baseline.

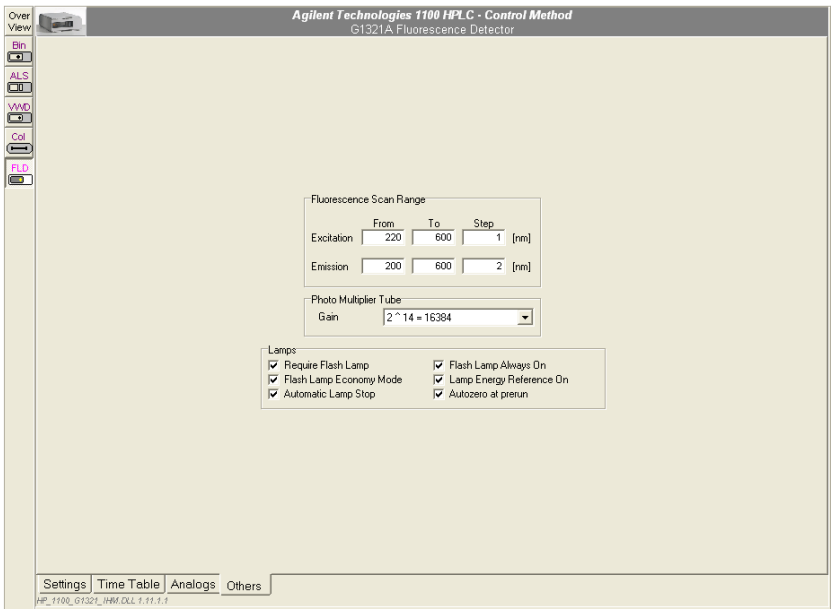
In the Attenuation scrolling list, select the attenuation value. The available values are: 0.195 LU, 0.391 LU, 0.781 LU, 1.563 LU, 3.125 LU, 6.25 LU, 12.5 LU, 25 LU, 50 LU, 100 LU, 200.00 LU, 400.00 LU, 800.00 LU, 1600.00 LU.

In the Range scrolling list, enter the output voltage range value. The available values are: 0.1 Volt Full Scale and 1 Volt Full scale.

In the Source scrolling list, select the type of the collected signal. The available choices are: EX1/EM1, EM2/EX2, EM3/EX3, EM4/EX4, sample w/o reference, Reference without sample, Raw sample, Raw reference, Test chromatogram, Analog output test, Board temperature.

Select the Polarity of the detector.

Phosphorescence Control

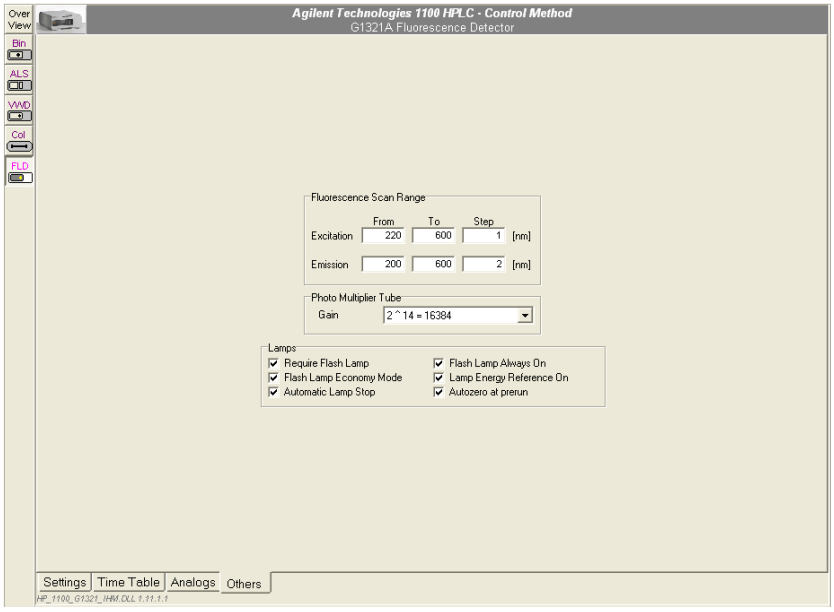


Settings Parameter Group

Enter the Delay in the corresponding field.

Enter the Gate in the corresponding field.

Others Control



Fluorescence Scan Range Parameter Group

In the fields Excitation/Emission From and Excitation/Emission To, enter the minimum and maximum wavelengths of the spectra.

Enter the Excitation/Emission Step in the corresponding field. A small wavelength step will enhance the spectrum resolution.

Photo Multiplier Tube Parameter Group

Select the value of the Gain parameter (amplification factor).

Lamps Parameter Group

Check Require Flash Lamp if necessary.

Flash Lamp Economy Mode decreases the frequency of the lamp flash.

Automatic Lamp Stop automatically stops the detector's lamp at the end of the run.

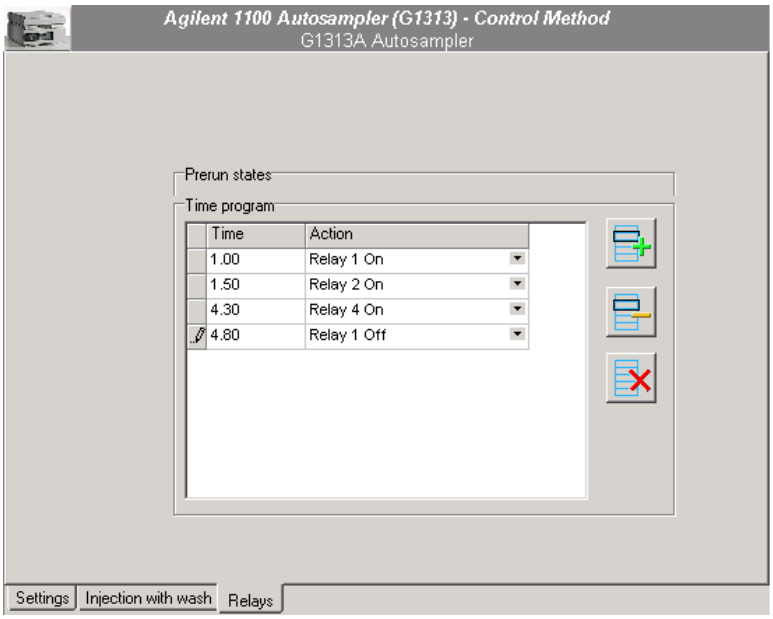
Flash Lamp Always On enables permanent flash mode.

Lamp Energy Reference On configures the signal as a reference.

Autozero At Prerun performs an autozero of the detector before the run.

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

Relay ON means the relay is closed.

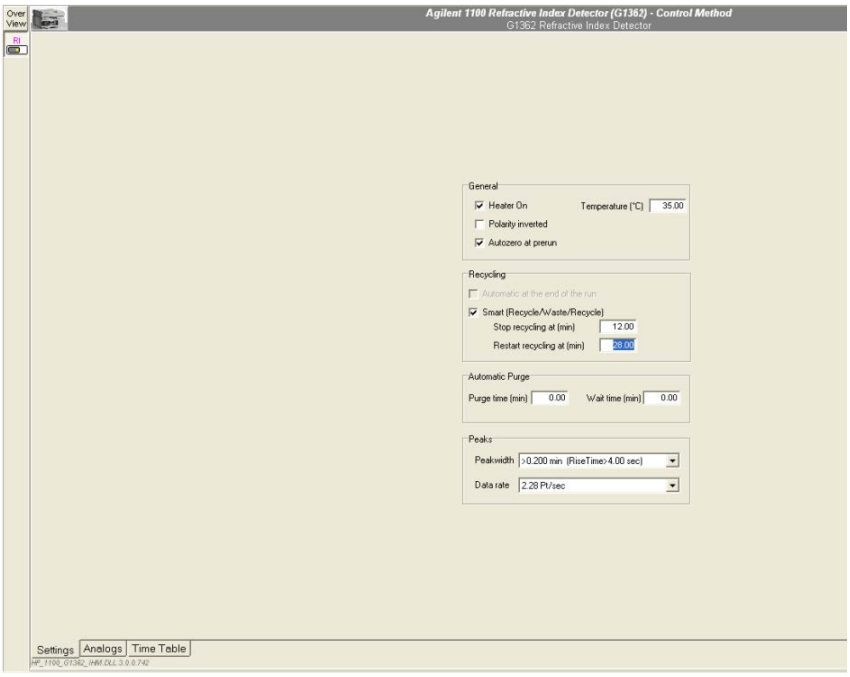
NOTE: If the chromatographic system is fitted out with both a G1321(FLD) and either a G1314 (VWD), a G1315 (DAD) or a G1365 (MWD), and that you want not the VWD/DAD/MWD lamp to be turned ON during acquisition (only FLD signal is required), you must first stop the VWD/DAD/MWD lamp (from status), then uncheck all the VWD/DAD/MWD channels in the acquisition method.

If VWD/DAD/MWD channels are unchecked in the method, the corresponding UV/Vis lamp state is not changed when lunching an acquisition. That means that if UV/Vis lamp is ON before starting the acquisition it will stayed ON during the acquisition, if it is OFF it will stayed OFF. This allows the user to spare the UV/Vis lamps of the VWD/DAD/MWD detectors.

Control Section for the Agilent LC 1260 Refractive Index Detector (G1362)

Click on the button to display the Agilent Technologies 1260Retention Index Detector (G1362) control method section. It contains three sub-sections: Settings, Analogs and Time table. Click on the required sub-section to define the corresponding parameters that will be used during the chromatographic run.

Settings Control



General Parameter Group

Check Heater On to turn the heater on.

In the Temperature field, enter the value of the optical unit Temperature.

Check Polarity inverted to invert the polarity.

Check Autozero at prerun to perform an autozero of the detector just before the run.

Recycling Parameter Group

Check Automatic at the end of the run to switch the recycle valve to the on position after one analysis has been completed and to return it to the off position before the next analysis starts.

Check Smart (Recycle/Waste/Recycle) to save mobile phase solvents.

In the Stop recycling at field, enter the time t1 (min) before the first peak is eluted in order to switch the recycle valve to the off position. Enter the time t2 (min) in the Restart recycling at field to switch the recycle valve to the off position as soon as the last chromatographic peak is eluted. As a consequence, mobile phase will be recycling until the end of the run and after. Note that it is mandatory that t1 < t2.

Automatic Purge Parameter Group

In the Purge time field, enter the time during which the instrument is purged.

In the Wait time field, enter the time to wait after a purge.

Peaks Parameter Group

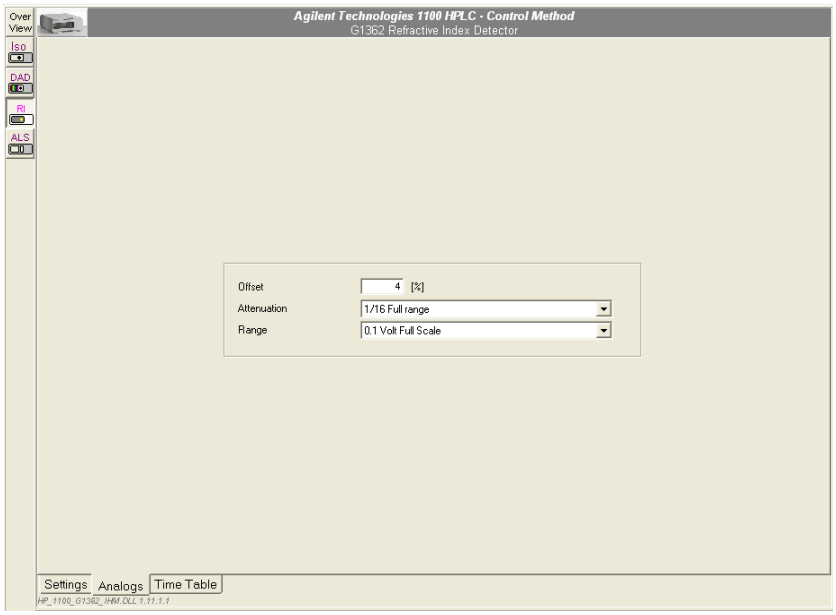
Select the Peakwidth value in the scrolling list. This parameter influences the peak detection. A response time is associated with each peakwidth value. The available values are:

<0.005 min (RiseTime<0.12 sec)
>0.005 min (RiseTime>0.12 sec)
>0.010 min (RiseTime>0.25 sec)
>0.025 min (RiseTime>0.5 sec)
>0.05 min (RiseTime>1 sec)
>0.1 min (RiseTime>2 sec)
>0.2 min (RiseTime>4 sec)
>0.4 min (RiseTime>8 sec)

Select the Data rate value in the scrolling list. This parameter is associated to the previous ones. The available values are:

36.50 Pt/sec
18.25 Pt/sec
9.12 Pt/sec
4.56 Pt/sec)
2.28 Pt/sec
1.14 Pt/sec

Analogs Control

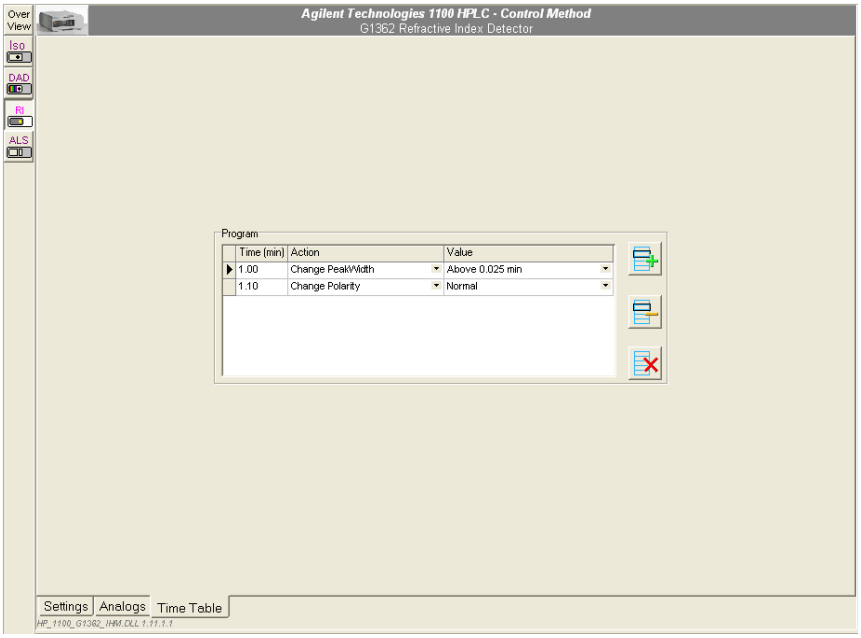


In the Offset field, enter the offset value to adjust the baseline.

In the Attenuation scrolling list, enter the attenuation value. The available values are: 1/1024 Full range, 1/512 Full range, 1/256 Full range, 1/128 Full range, 1/64 Full range, 1/32 Full range, 1/16 Full range, 1/8 Full range, ¼ Full range, ½ Full range, 1x Full range and 2x Full range.

In the Range scrolling list, enter the output voltage range value. The available values are: 0.1 Volt Full Scale and 1 Volt Full scale.

Time Table Control



Program Parameter Group

Program peakwidth and/or the polarity changes during the run. Use the following buttons to edit the table:

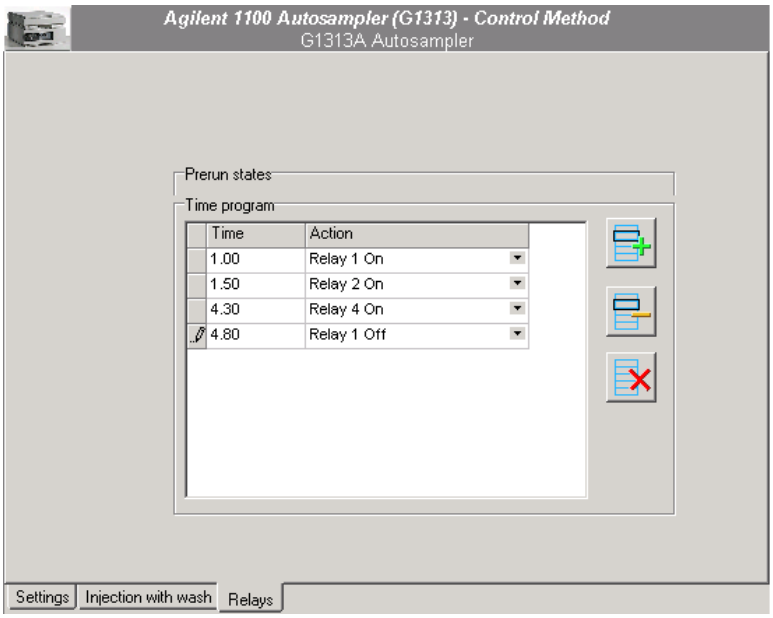
to add a line to the table.

to delete a line in the table.

to clear the entire table.

Relays tab

If a relay board option is configured, another tab is available:



User can define the relay program.

Relay ON means the relay is closed.

Starting and Viewing an Acquisition

Quick Start and Sequence

Once the instrument control method has been correctly programmed, an analysis can be started. The next section briefly describes how to start an acquisition.

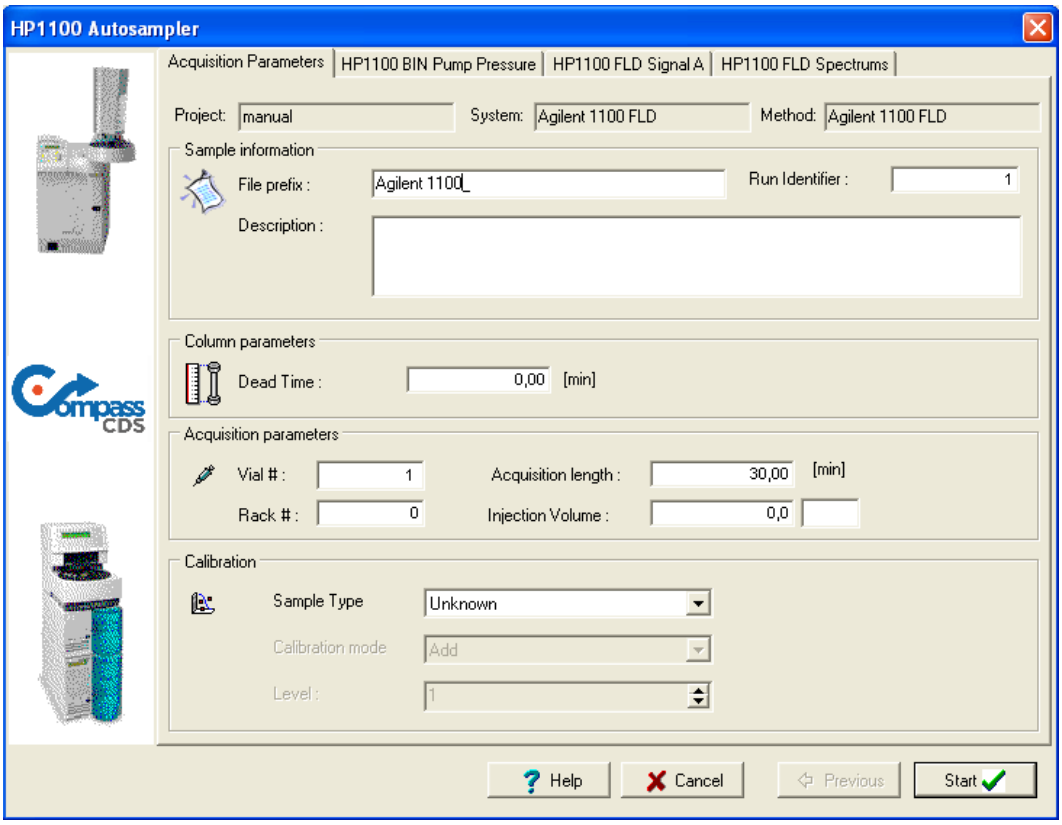
Quick Start (Single Acquisition)

Press the button.

In the Quick Start window, select the system, the method and optionally the project if connected in "All project" mode.

Press the OK button.

The following screen is displayed:



In the Acquisition parameters tab, required fields like the Run Name, the Run ID and the Acquisition length must be filled in before starting an analysis. Furthermore, if the system is equipped with an autosampler controlled by the CompassCDS Chromatography Data System, the Injection Volume, the Vial position and the Rack number (if required) must be entered.

Other parameters associated with each acquisition channel can be entered in the Channel X tab.

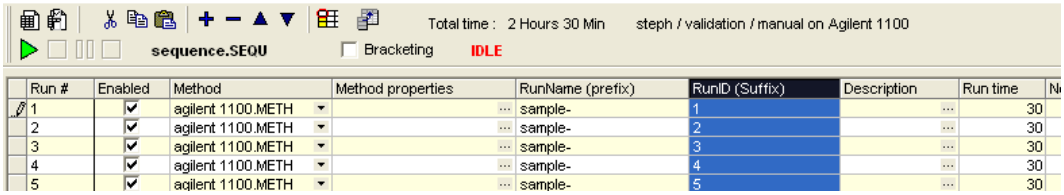
Click on the Start button to start the acquisition if the system is a single-injector system or click on the Next button if the system is a multiple injector system. In a multiple injector system, the same

parameters entered for the first injector must be entered for the other injectors before starting the acquisition.

Sequence

To create a sequence, select the FILE / NEW SEQUENCE menu, and complete the displayed creation wizard screen (refer to the CompassCDS Chromatography Data System User's Guide), by entering the system name that will perform the analysis, the number of lines (corresponding to the number of samples), and the sequence name.

The sequence is displayed. Complete the sequence information columns (refer to the CompassCDS Chromatography Data System User's Guide).



Run #	Enabled	Method	Method properties	RunName (prefix)	RunID (Suffix)	Description	Run time
1	☑	agilent 1100.METH	...	sample-	1	...	30
2	☑	agilent 1100.METH	...	sample-	2	...	30
3	☑	agilent 1100.METH	...	sample-	3	...	30
4	☑	agilent 1100.METH	...	sample-	4	...	30
5	☑	agilent 1100.METH	...	sample-	5	...	30

The Method Name, the Run Name, the Run ID, and the Acquisition length must be filled in before starting the analysis. All these parameters are automatically imported from the acquisition part if defined in the method.

Start the sequence by clicking on the button.

NOTE: For more details about how to start an acquisition, refer to the CompassCDS Chromatography Data System User's Guide.

Running Acquisition Status

Viewing a Running Acquisition

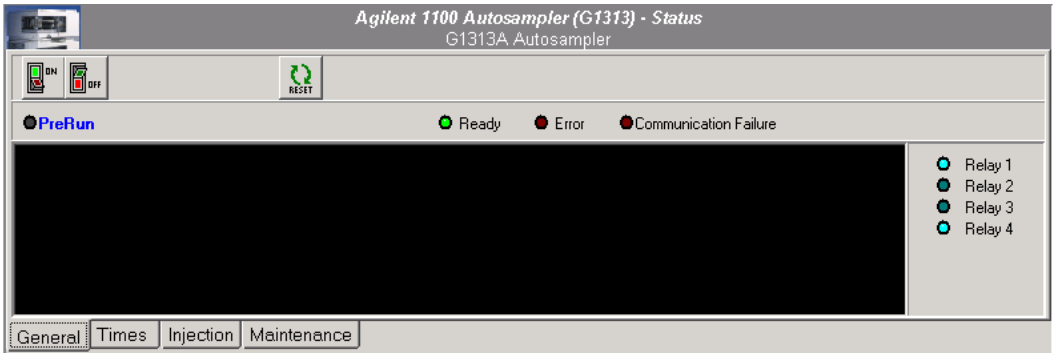
To view a running acquisition, click on the Systems tab, then select the running system. A window is activated which is composed of two parts: the running chromatogram and the status window where the driver modules are listed.

Status of the Agilent LC 1260 Autosampler (G1313)

Click on the

button to display the Agilent Technologies 1260 Autosampler (G1313) status screen. It contains four sub-sections: General, Times, Injection and Maintenance. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the autosampler.

Information about the autosampler status is displayed: Faults, not ready parameters, etc.

If a relay/BCD board is installed, the relay states are displayed on the left part of the screen.

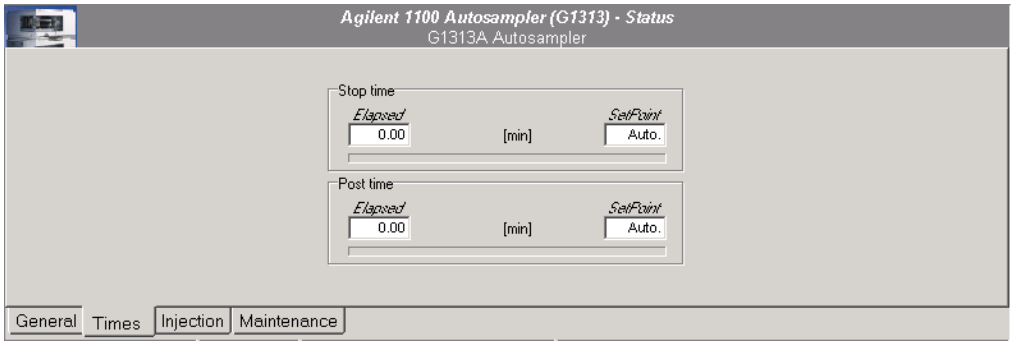
The button turns on all the system modules.

The button turns off all the system modules.

The button reset the autosampler.

The LED gives information about the general status of the autosampler: Communication failure, Start Up, Error, and Ready.

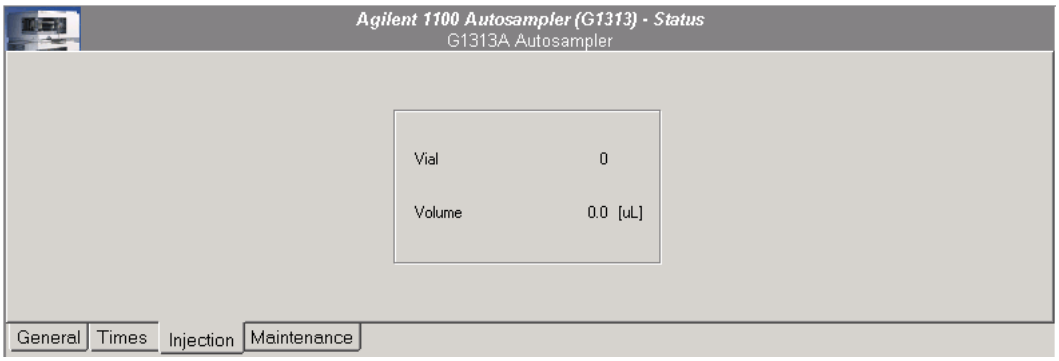
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

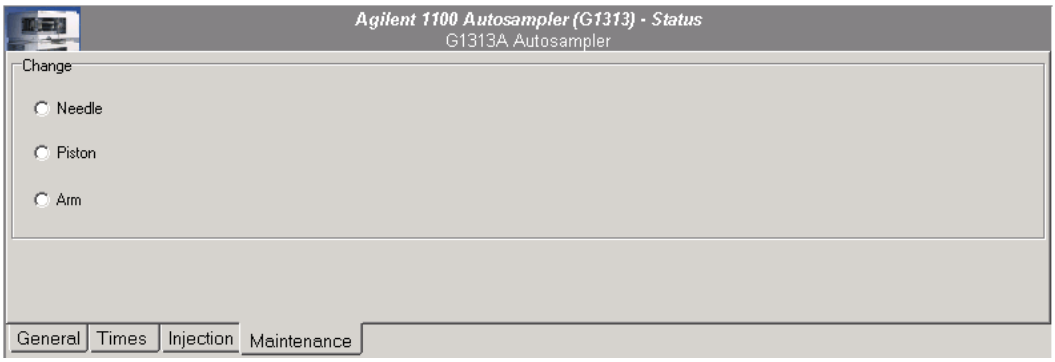
Injection Window



This is a read-only window.

The vial and the injection volume are displayed.

Maintenance Window



This window is used for maintenance operation on the autosampler.

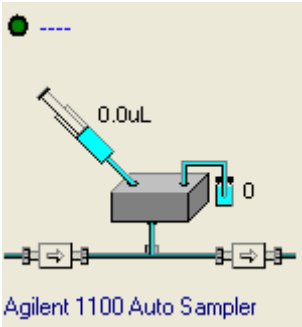
Select with the radio button on which part of the instrument the maintenance will be done and press the Change button. Three choices are available: Needle, Piston and Arm.

When the maintenance is complete, press the Done button.

Overview Window

Click on the Over View button: the Status Overview window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, vial injected and volume injected).



Not ready: contains the not ready information sent by the instrument.

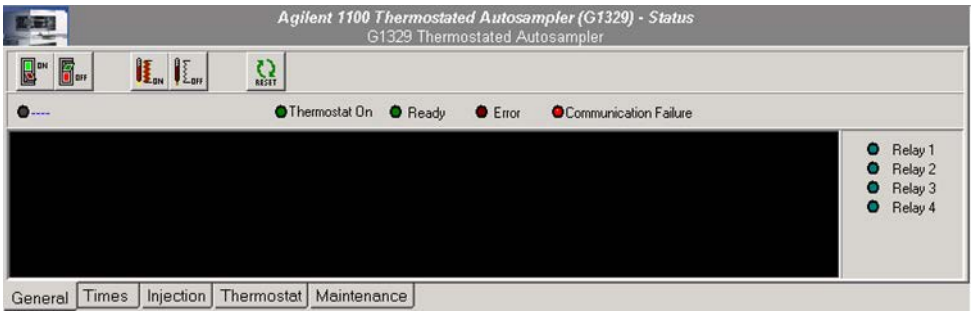
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Thermostated Autosampler (G1329)

Click on the

button to display the Agilent Technologies 1260 Thermostated Autosampler (G1329) status screen. It contains five sub-sections: General, Times, Injection, Thermostat, and Maintenance. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the autosampler.

Information about the autosampler status is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button turns on the thermostat.

The

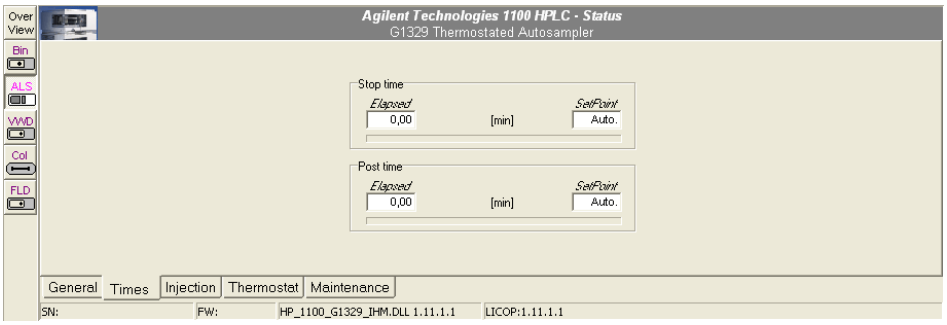
button turns off the thermostat.

The

button reset the autosampler.

The LEDs give information about the general status of the instrument: Communication failure, Error, Ready, etc.

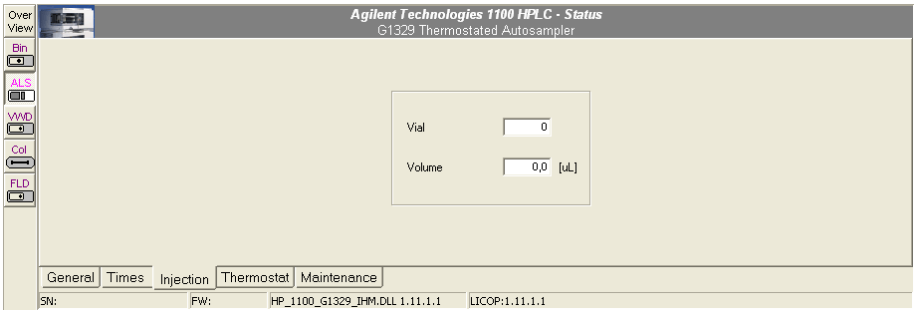
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

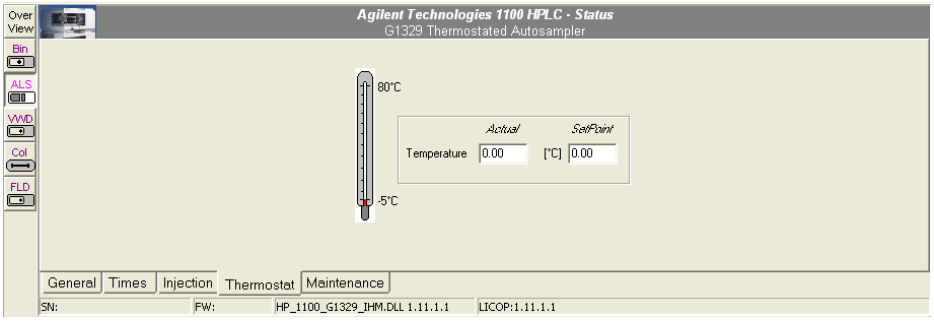
Injection Window



This is a read-only window.

The vial and the injection volume are displayed.

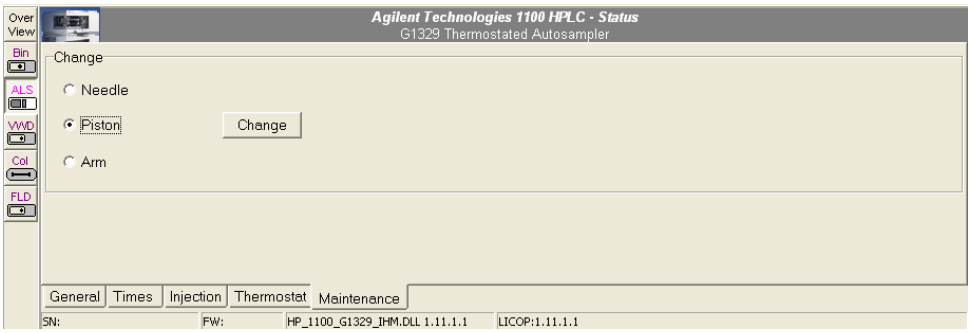
Thermostat Window



This is a read-only window.

The actual temperature and the setpoint temperature of the heated area are displayed.

Maintenance Window



This window is used for maintenance operation on the autosampler.

Select with the radio button on which part of the instrument the maintenance will be done and press the Change button. Three choices are available: *Needle, Piston* and *Arm.*

When the maintenance is complete, press the Done button.

Overview Window

Click on the Over View button: the ***Status Overview*** window is displayed and contains three tabs:

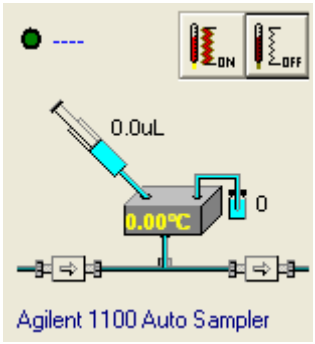
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, vial injected, temperature and volume injected).

The

button turns on the thermostat.

The

button turns off the thermostat.



Not ready: contains the not ready information sent by the instrument.

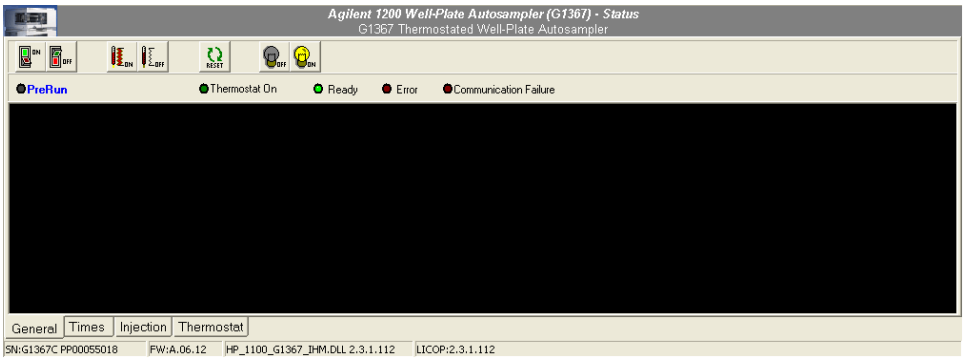
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Well Plate Autosampler (G1367)

Click on the

button to display the Agilent Technologies 1260Well Plate Autosampler (G1367) status screen. It contains four sub-sections: *General, Times, Injection,* and *Thermostat*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the autosampler.

Information about the autosampler status is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button reset the autosampler.

The

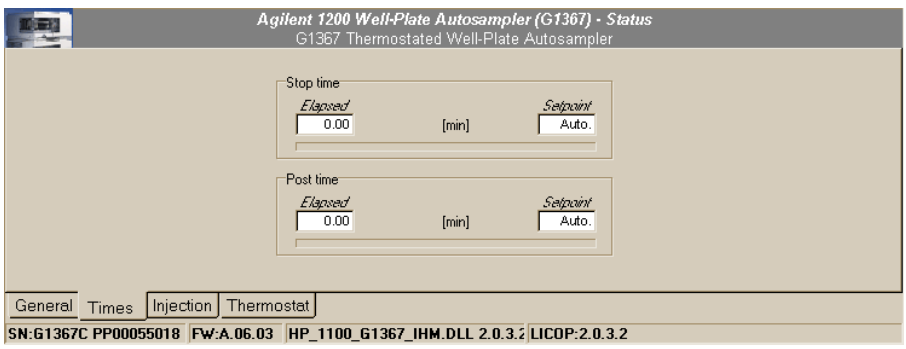
button turns on the thermostat.

The

button turns off the thermostat.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

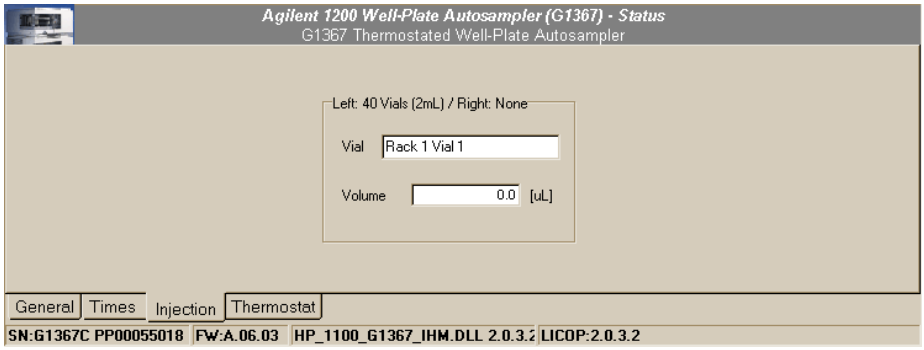
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

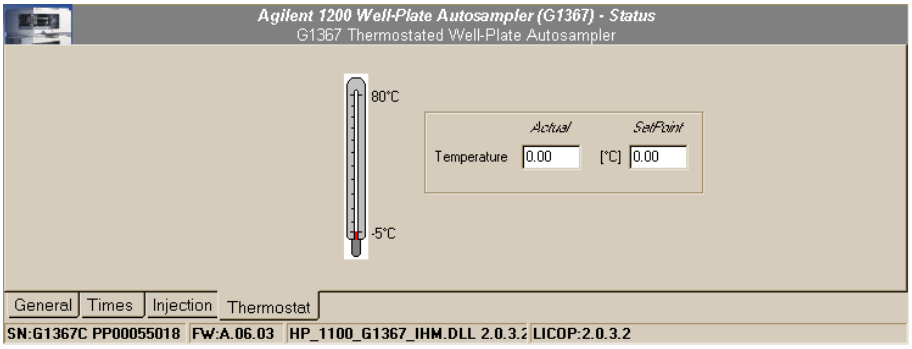
Injection Window



This is a read-only window.

The vial and the injection volume are displayed.

Thermostat Window



This is a read-only window.

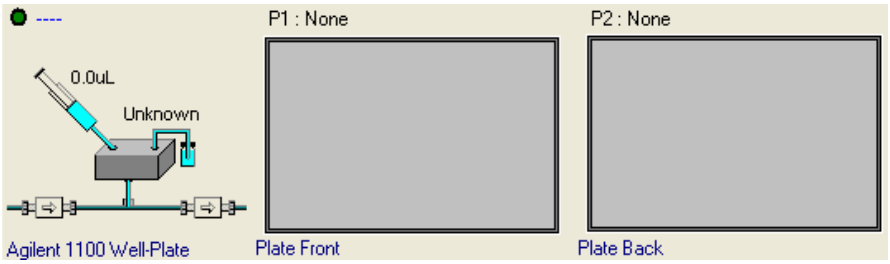
The actual temperature and the set point temperature of the heated area are displayed.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, vial injected, temperature and volume injected).



Not ready: contains the not ready information sent by the instrument.

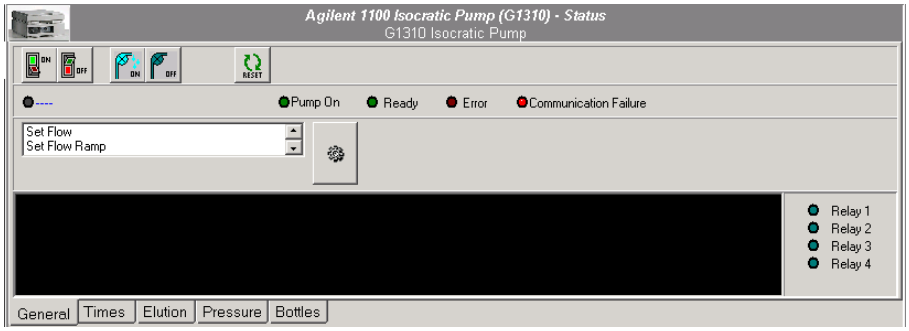
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Isocratic Pump (G1310)

Click on the

button to display the Agilent Technologies 1260Isocratic Pump (G1310) status screen. It contains five sub-sections: *General, Times, Elution, Pressure,* and *Bottle*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the pump.

Information about the pump is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button turns on the pump module only.

The

button turns off the pump module only.

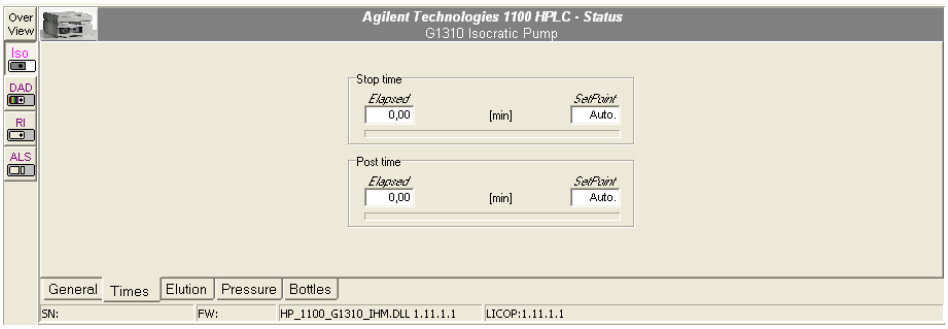
The

button reset the pump module.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

By clicking on *Set Flow* or *Set Flow Ramp*, another field will appear allowing you to modify the current values. Apply the new values with the button.

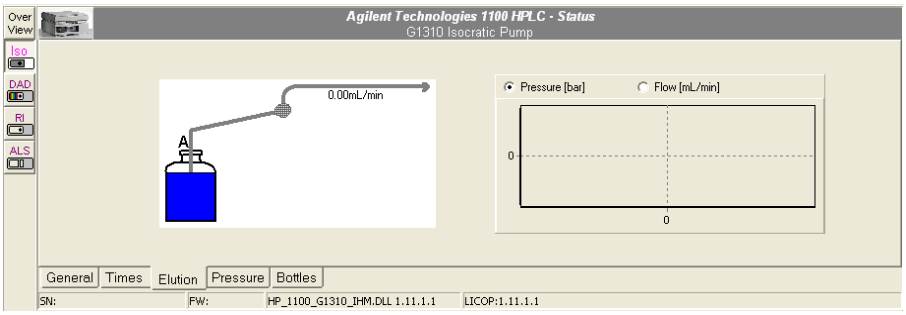
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

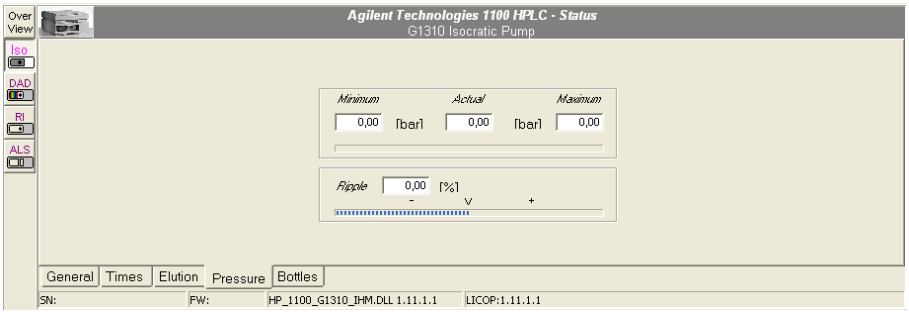
Elution Window



This is a read-only window.

The actual flow rate and the pressure evolution or the flow evolution is displayed in this screen, according to the user choice.

Pressure Window

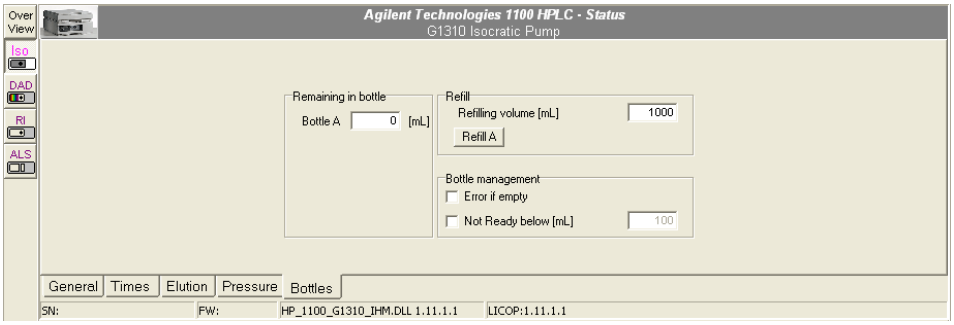


This is a read-only window.

The *Minimum, Actual* and *Maximum* pressures are displayed.

The *Ripple* value is also displayed.

Bottles Window



Remaining in Bottle Parameter Group

The remaining volume of the bottle is indicated in the field *Bottle A*.

Refill Parameter Group

Enter the *Refilling volume* and click on *Refill A* to refill the bottle A.

Bottle Management Parameter Group

Check *Error if empty* to place the Agilent Technologies 1260 in error state when the eluent bottle is empty.

Check *Not Ready Below* to place the instrument in not ready mode when the remaining volume is less than the entered value.

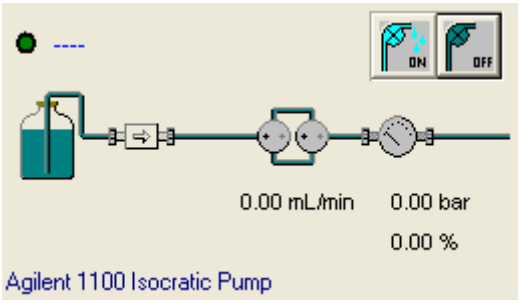
Overview Window

Click on the Over View button: the ***Status Overview*** window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, pressure, ripple and flow).

The ON button turns on the pump module only.

The OFF button turns off the pump module only.



Not ready: contains the not ready information sent by the instrument.

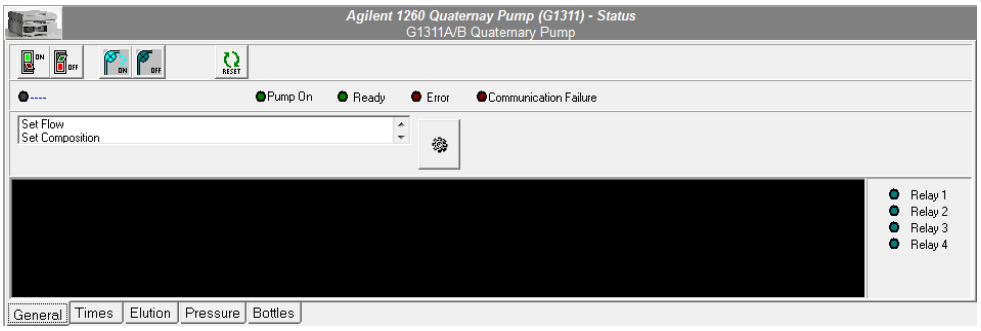
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Quaternary Pump (G1311)

Click on the

button to display the Agilent Technologies 1260Quaternary Pump (G1311 and G5611 modules) status screen. It contains five sub-sections: *General, Times, Elution, Pressure,* and *Bottles*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the pump.

Information about the pump status is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button turns on the pump module only.

The

button turns off the pump module only.

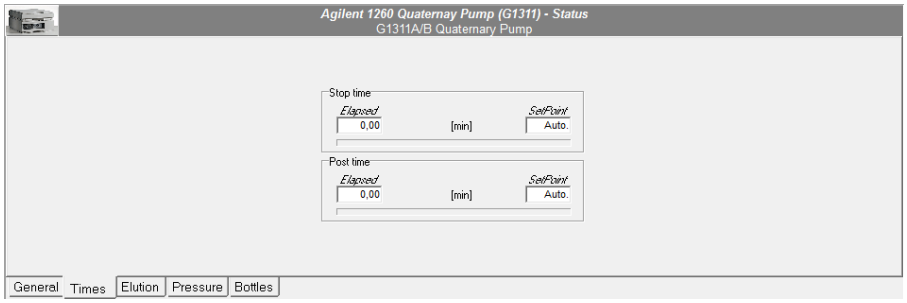
The

button reset the pump module.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

By clicking on *Set Flow, Set Composition*, *Set Flow Ramp, Turn Seal wash Off or Active Single Seal Wash,* another field will appear allowing you to modify the current values. Apply the new values with the
button.

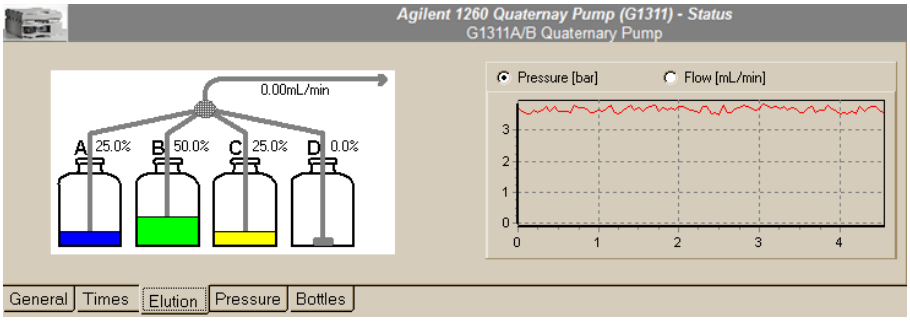
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

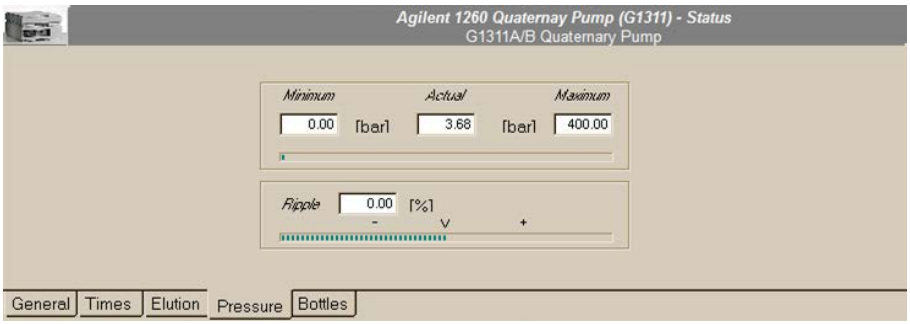
Elution Window



This is a read-only window.

The actual flow rate and the percentages of each solvent in the mobile phase are displayed. According to the user choice, the pressure or the flow evolution is plotted against time in this screen.

Pressure Window

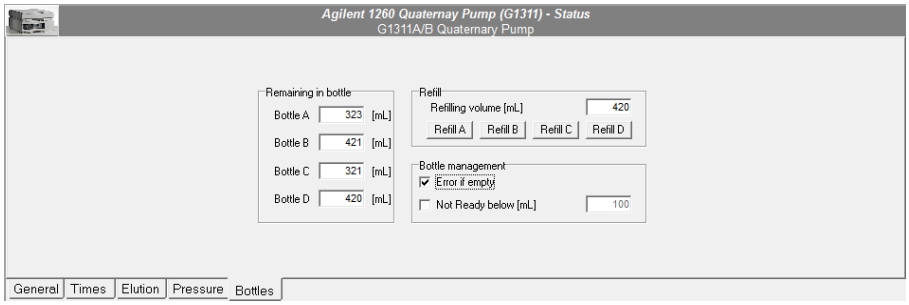


This is a read-only window.

The *Minimum, Actual* and *Maximum* pressures are displayed.

The *Ripple* value is also displayed.

Bottles Window



Remaining in Bottle Parameter Group

The remaining volume of each bottle is indicated in the fields *Bottle A, Bottle B, Bottle C and Bottle D*.

Refill Parameter Group

Enter the *Refilling volume* and click on *Refill* button to refill each bottle.

Bottle Management Parameter Group

Check *Error if empty* to place the Agilent Technologies 1260in error state when the eluent bottle is empty.

Check *Not Ready Below* to place the instrument in not ready mode when the remaining volumes are less than the values entered.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

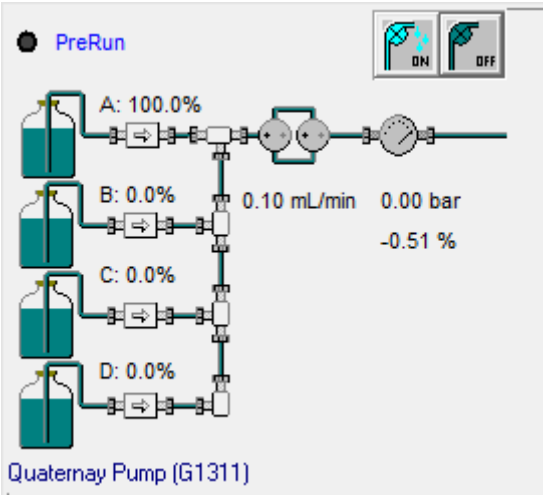
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, pressure, ripple and flow).

The

button turns on the pump module only.

The

button turns off the pump module only.



Not ready: contains the not ready information sent by the instrument.

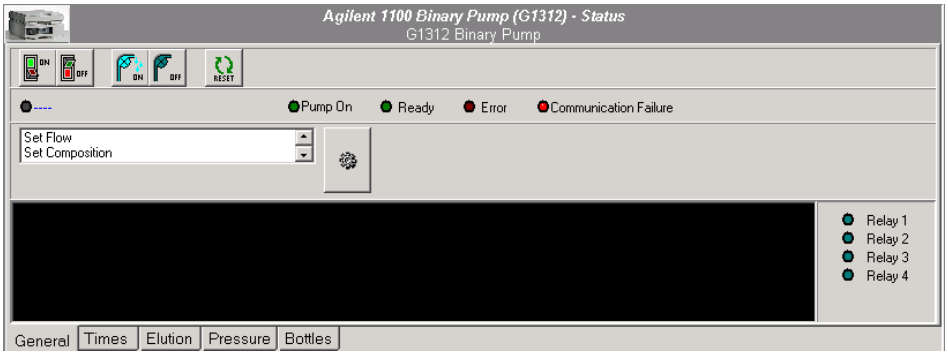
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Binary Pump (G1312)

Click on the

button to display the Agilent Technologies 1260Binary Pump (G1312) status screen. It contains five sub-sections: *General, Times, Elution, Pressure,* and *Bottles*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the pump.

Information about the pump status is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button turns on the pump module only.

The

button turns off the pump module only.

The

button reset the pump module.

The

button activates the A1 channel of the Solvent Selection Valve A.

The

button activates the A2 channel of the Solvent Selection Valve A.

The

button activates the B1 channel of the Solvent Selection Valve B.

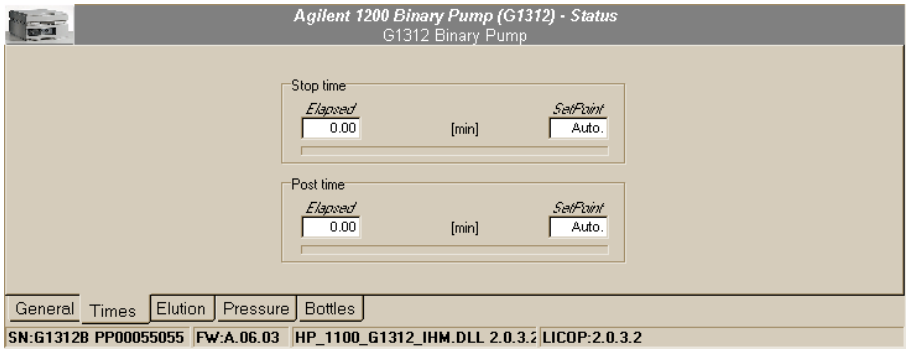
The

button activates the B2 channel of the Solvent Selection Valve B.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

By clicking on *Set Flow*, *Set Composition* Set flow ramp, Turn Seal Wash Off, Active Single Seal Wash or Active Periodic Seal Wash, another field will appear allowing you to modify the current values. Validate the new values with the button.

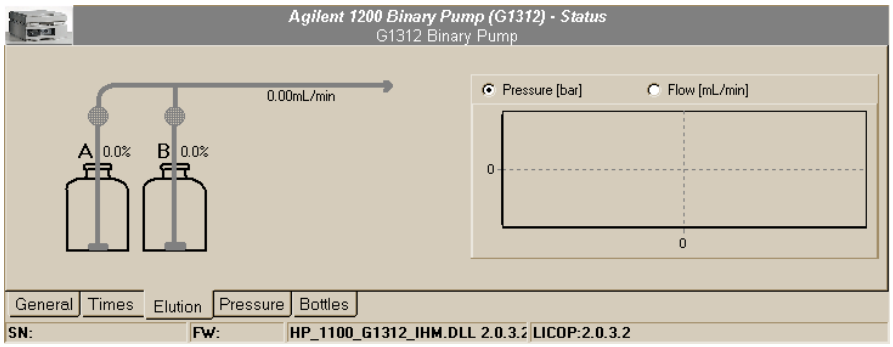
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

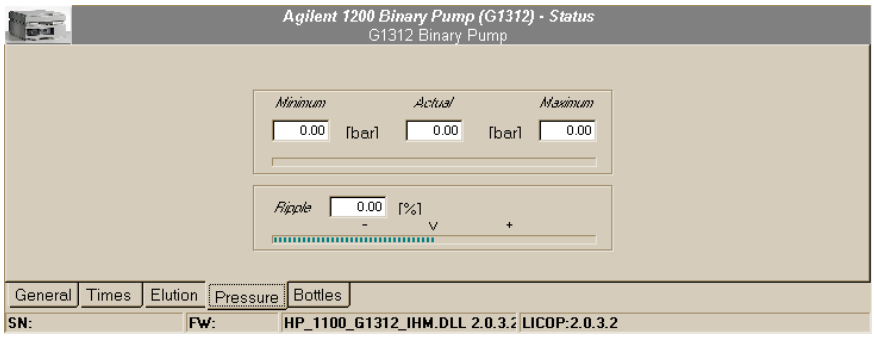
Elution Window



This is a read-only window.

The actual flow rate and the percentages of each solvent in the mobile phase are displayed. According to the user choice, the pressure or the flow is plotted against time on this screen.

Pressure Window

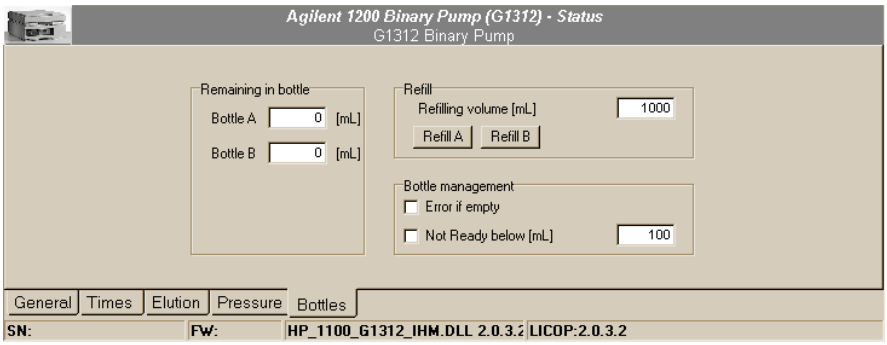


This is a read-only window.

The *Minimum, Actual* and *Maximum* pressures are displayed.

The *Ripple* value is also displayed.

Bottles Window



Remaining in Bottle Parameter Group

The remaining volume of each bottle is indicated in the fields *Bottle A and Bottle B*.

Refill Parameter Group

Enter the *Refilling volume* and click on *Refill* to refill each bottle.

Bottle Management Parameter Group

Check *Error if empty* to place the Agilent Technologies 1260 in error state when the eluent bottle is empty.

Check *Not Ready Below* to place the instrument in not ready mode when the remaining volumes are less than the values entered.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

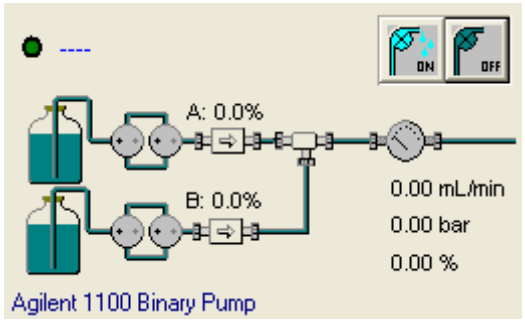
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, pressure, ripple and flow).

The

button turns on the pump module only.

The

button turns off the pump module only.



Not ready: contains the not ready information sent by the instrument.

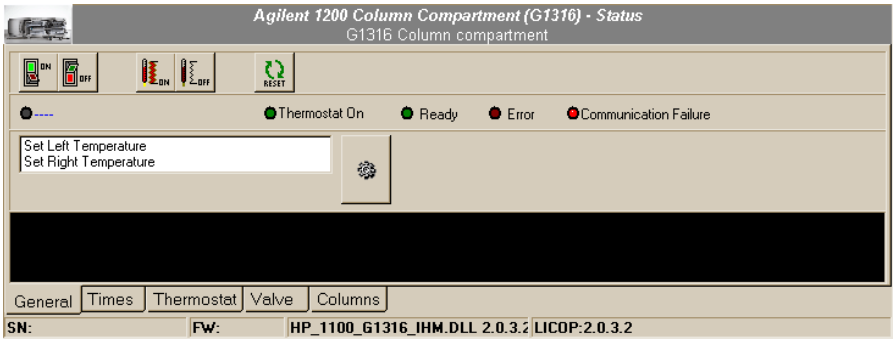
Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Column Compartment (G1316)

Click on the

button to display the Agilent Technologies 1260 Column Compartment (G1316) status screen. It contains five sub-sections: *General, Times, Thermostat, Valve,* and *Columns*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the column compartments.

Information about the column compartment status is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The button turns off all the system modules.

The button turns on the column compartment heater.

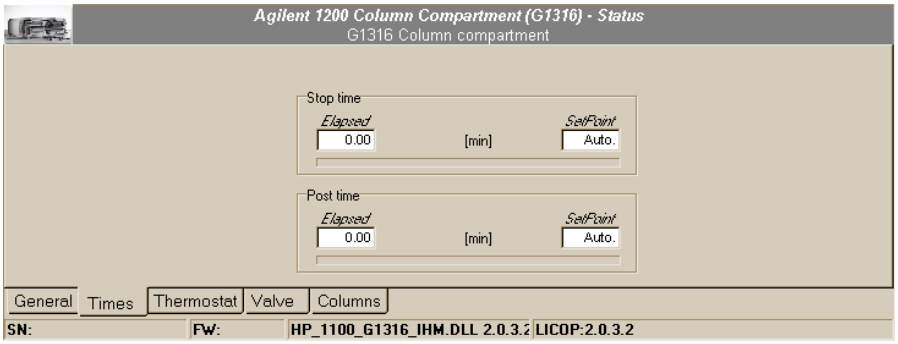
The button turns off the column compartment heater.

The button reset the column compartment heater.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc. The thermostat is displayed as ON if OFF is sent by a method (direct download or acquisition, because if not, the thermostat will never be ready.*

Select *Set Left (*or *Right) temperature*, then enter the desired temperature in the *Left (*or *Right) temperature* field and click on the button to send the new temperature to the instrument.

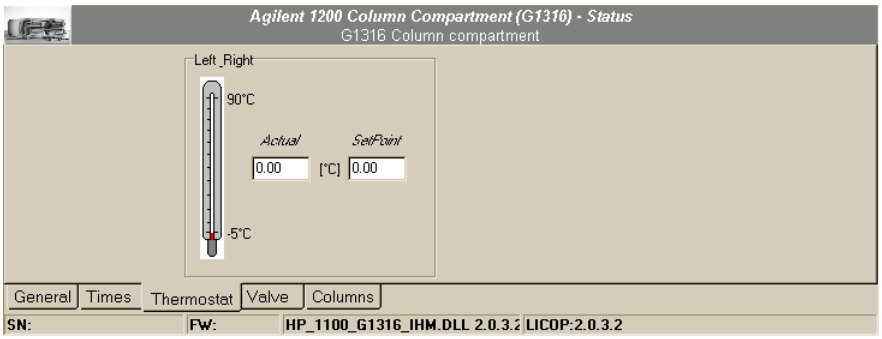
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed

Thermostat Window

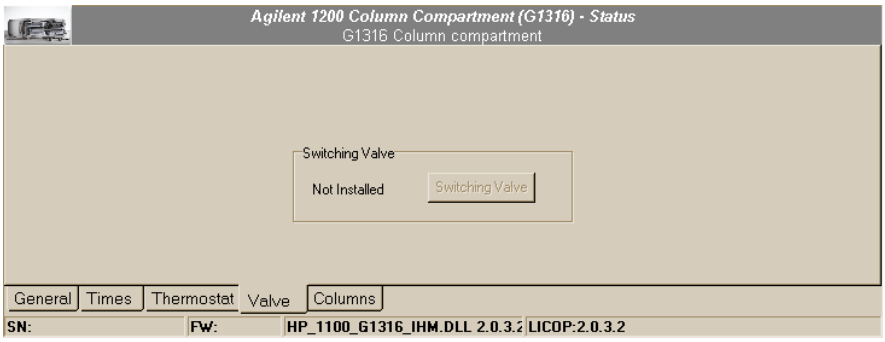


This is a read-only window.

The actual and setpoint temperatures for the right and left compartments are displayed.

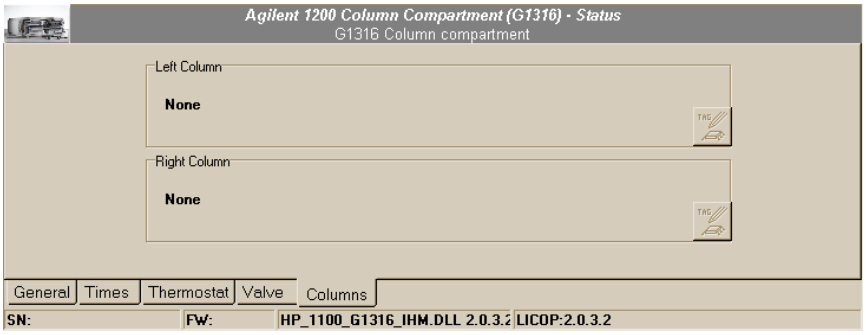
When sending a method with one or both thermostats OFF, the setpoint displayed on this screen is OFF. On the General tab, the thermostat is still displayed as ON, because if not, the thermostat will never be ready.

Valve Window



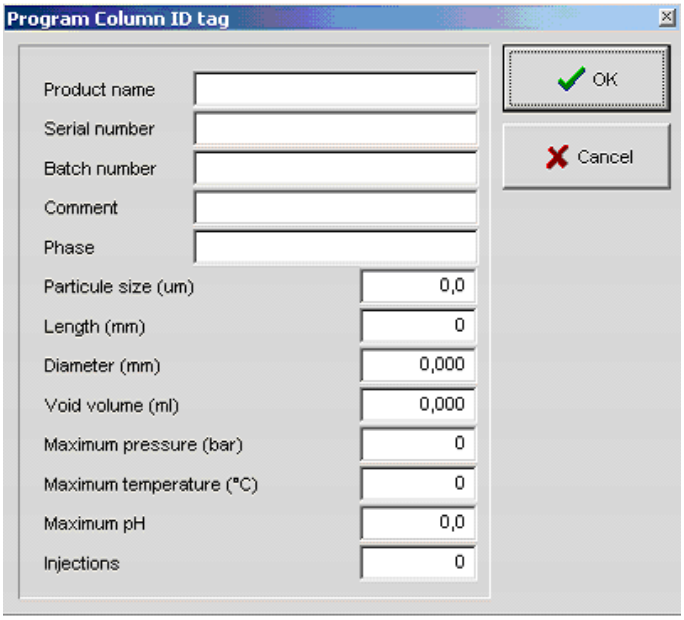
The current valve position is displayed and can be changed from this screen.

Column Window



The current tagID properties are displayed and can be changed from this screen.

To program the tagID, press the button. The following screen is displayed that allows the user to program the tagID.



Please note that the *Injections* field is automatically incremented by one after each injection of the system.

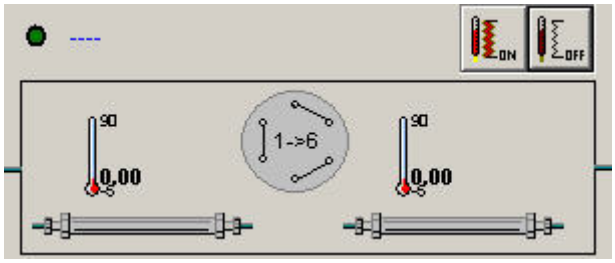
Overview Window

Click on the Over View button: the ***Status Overview*** window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, temperatures and valve position).

The ON button turns on the column compartment heater.

The OFF button turns off the column compartment heater.



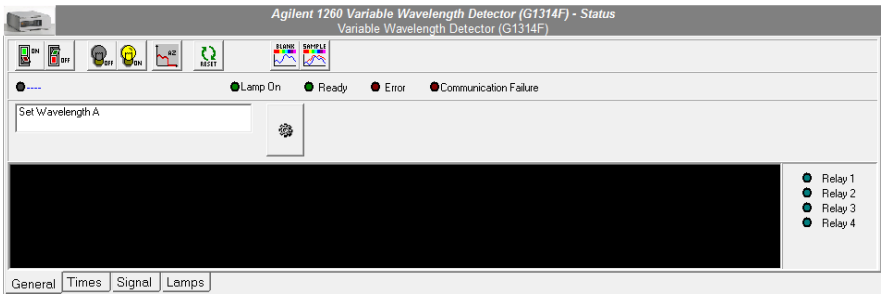
Not ready: contains the not ready information sent by the instrument.

Events: contains the events that have occurred on the instrument.

Status of the Agilent LC 1260 Variable Wavelength Detector (G1314)

Click on the button to display the Agilent Technologies 1260Variable Wavelength Detector (G1314) status screen. It contains four sub-sections: *General, Times, Signal*, and *Lamps*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the detector.

Information about the detector status is displayed: Faults, not ready parameters, etc.

The button turns on all the system modules.

The button turns off all the system modules.

The button switches on the detector lamp.

The button switches off the detector lamp.

The button defines a blank spectrum. This spectrum will be subtracted from the sample spectrum.

The button allows the user to define a sample spectrum. If a blank spectrum has been defined, it will be subtracted to the sample spectrum.

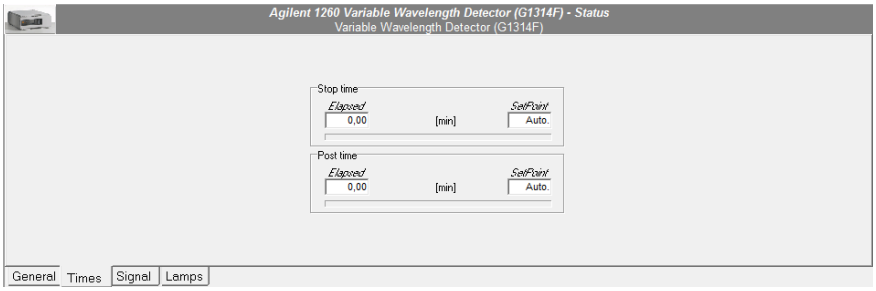
The button autozeros the detector.

The button reset the detector module.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

Select *Set Wavelength A*, then enter the desired Wavelength in the *Wavelength* field and click on the button to send the new wavelength to the instrument.

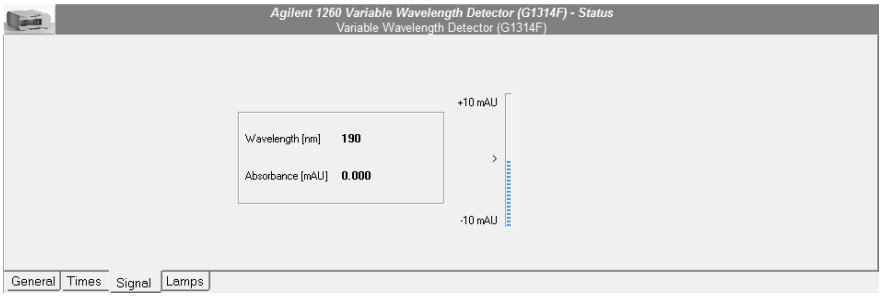
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

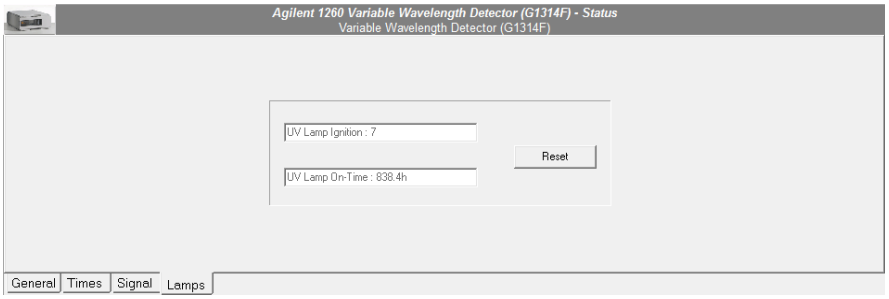
Signal Window



This is a read-only window.

The current wavelength and absorbance are displayed.

Lamps Window



This is a read-only window.

The UV Lamp Ignition and On-Time are displayed.

When the lamp is changed, reset the counters by pressing the reset button.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

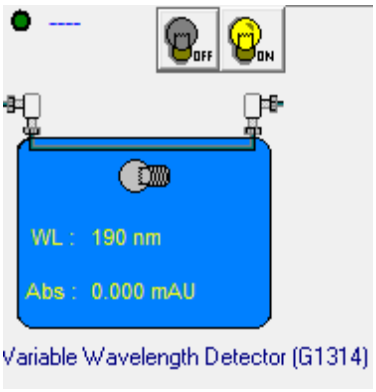
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, wavelength and absorbance).

The

button switches on the detector lamp.

The

button switches off the detector lamp.



Not ready: contains the not ready information sent by the instrument.

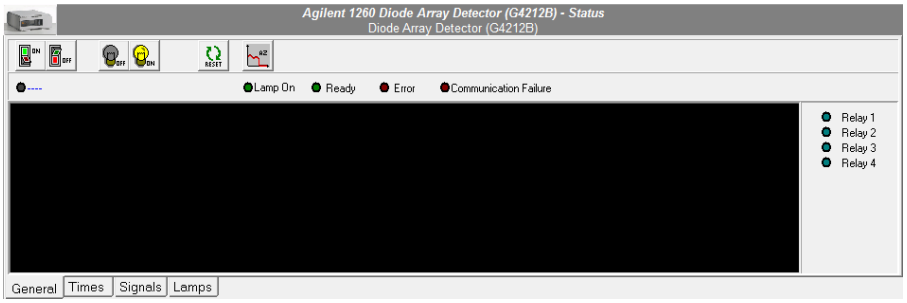
Events: contains the events that have occurred on the instrument.

Status of the Agilent Technologies 1260 LC Diode Array Detector (G1315 and G4212B) and of the Agilent Technologies 1260 Multiple Wavelength Detector (G1365)

Click on the

button to display the Agilent Technologies 1260LC Diode Array Detector (G1315 or G4212B) or the Agilent Technologies 1260 Multiple Wavelength Detector (G1365) status screen. It contains four sub-sections: *General, Times, Signals,* and *Lamps*. Click on the required sub-section to display the corresponding screen.

General Window



This window allows direct control of the detector.

Information about the detector status is displayed: Faults, not ready parameters, etc.

The button turns on all the system modules.

The button turns off all the system modules.

The button switches on the detector lamp.

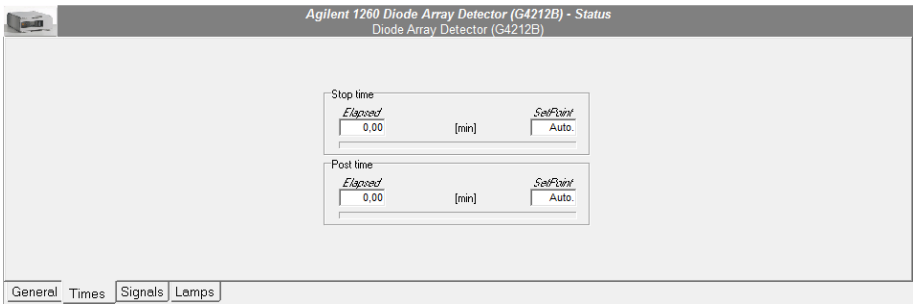
The button switches off the detector lamp.

The button reset the detector module.

The button autozeros the detector.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

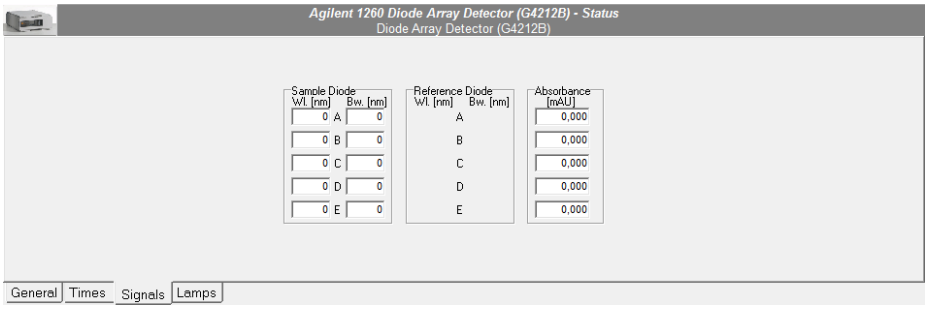
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

Signals Window

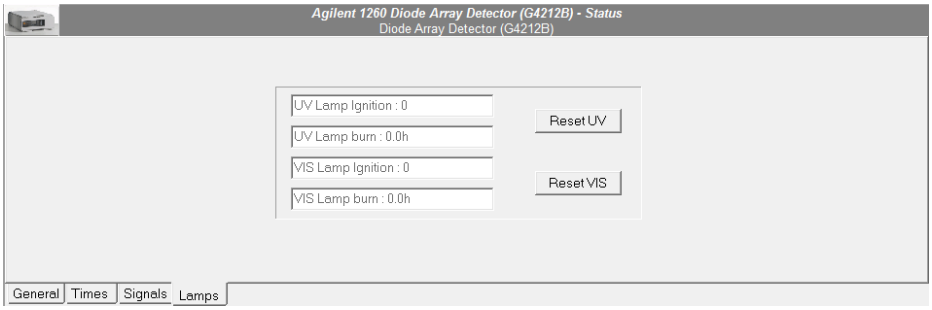


In the *Sample Diode* field are displayed the working wavelengths (*Wl*) and their bandwidths (*Bw*) for each channel.

The *Reference Diode* field showing the reference wavelengths and their bandwidths for each channel is not active.

The *Absorbance* field displays the current absorbance values of each channel.

Lamps Window



The *UV* and *VIS Lamp Ignition* and *burn* are displayed.

When a lamp is changed, reset the counters by pressing the *Reset UV* or *Reset VIS* button.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

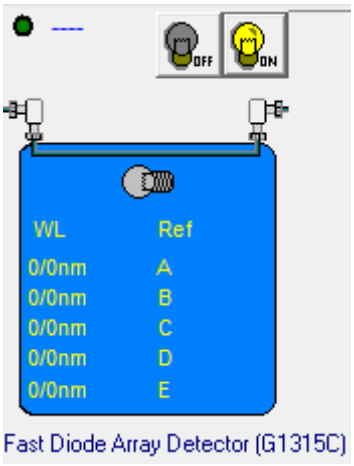
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, wavelength and absorbance).

The

button switches on the detector lamp.

The

button switches off the detector lamp.



Not ready: contains the not ready information sent by the instrument.

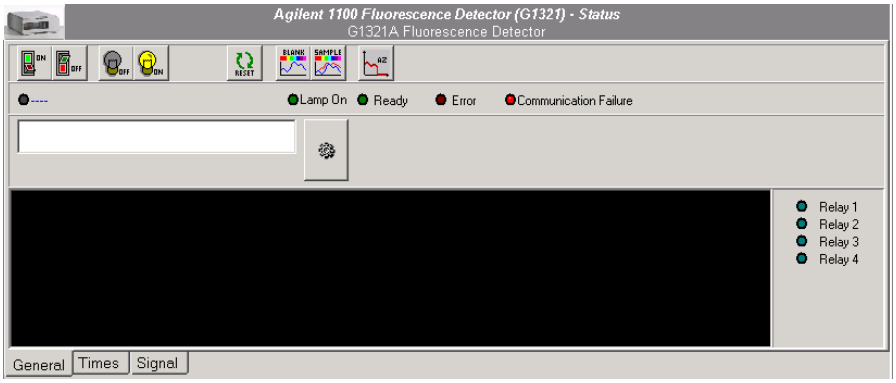
Events: contains the events that have occurred on the instrument.

Status of the Agilent Technologies 1260 Fluorescence Detector (G1321)

Click on the

button to display the Agilent Technologies 1260 Fluorescence Detector (G1321) status screen. It contains three sub-sections: *General, Times,* and *Signal*. Click on the required sub-section to display the corresponding screen.

General Window



Information about the detector is displayed: Faults, not ready parameters, etc.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button switches on the detector lamp.

The

button switches off the detector lamp.

The

button reset the detector module.

The

button and

button enables to take spectra. *Blank* defines the spectrum as a baseline spectrum which will be automatically subtracted to the other spectra (*Sample* button).

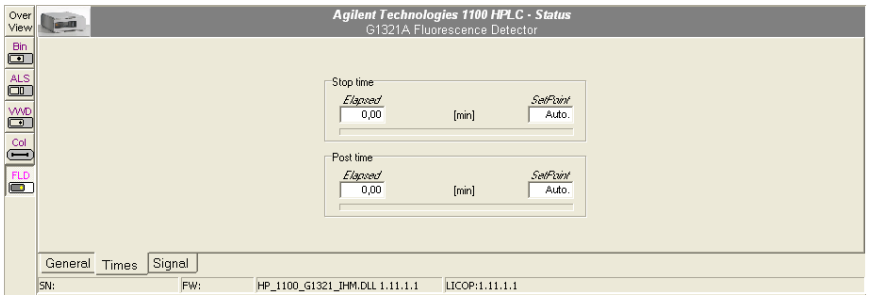
The

button autozeros the detector.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

The
button and the corresponding date entry area are not active for this detector.

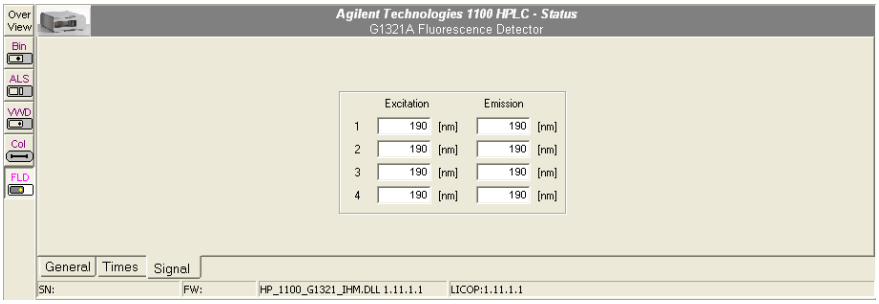
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

Signal Window



This is a read-only window.

The current *Excitation* and *Emission* wavelengths are displayed for each channel.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

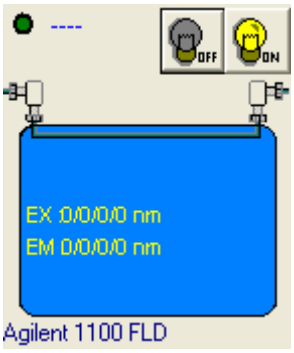
General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, wavelength and absorbance).

The

button switches on the detector lamp.

The

button switches off the detector lamp.



Not ready: contains the not ready information sent by the instrument.

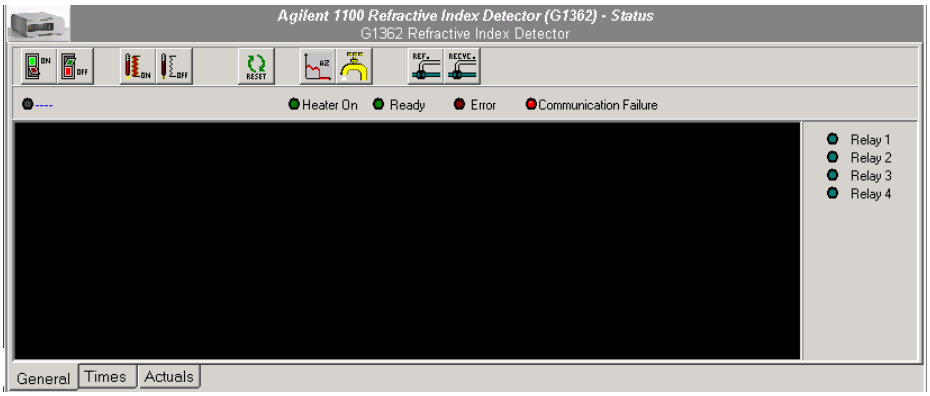
Events: contains the events that have occurred on the instrument.

Status of the Agilent Technologies 1260 Refractive Index Detector (G1362)

Click on the

button to display the Agilent Technologies 1260 Refractive Index Detector (G1362) status screen. It contains three sub-sections: *General, Times,* and *Actuals*. Click on the required sub-section to display the corresponding screen.

General Window



Information about the detector is displayed: Faults, not ready parameters, etc.

This window allows direct control of the detector.

The

button turns on all the system modules.

The

button turns off all the system modules.

The

button switches on the thermostat.

The

button switches off the thermostat.

The

button reset the detector module.

The button autozeros the detector.

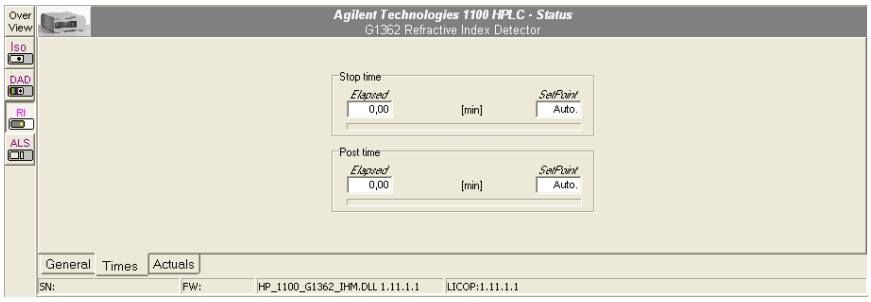
The button switches on the purge valve.

The button displays the reference valve control parameters. The available valve positions are: *Sample cell only* and *Reference and sample cells.* This action can be infinite or can begin at a precise time.

The button displays the recycle valve control parameters. The available valve positions are: *Cell to waste* and *Cell to solvent reservoir.* This action can be infinite or can begin at a precise time.

The LEDs give information about the general status of the instrument: *Communication failure, Error, Ready, etc.*

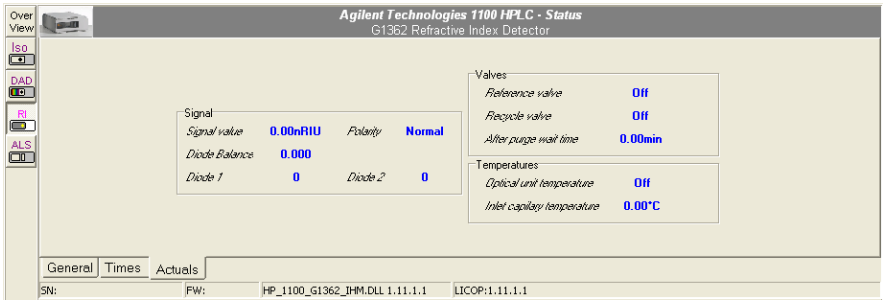
Times Window



This is a read-only window.

The elapsed run time and the elapsed post run time (if any) are displayed.

Actuals Window



This is a read-only window.

The current *Signal* parameters, the current *Valves* states and the major *Temperatures* are displayed.

Overview Window

Click on the

button: the ***Status Overview*** window is displayed and contains three tabs:

General: displays the synopsis of the instrument, where some current values can be read (state of the instrument, wavelength and absorbance).

The

button switches on the thermostat.

The

button switches off the thermostat.

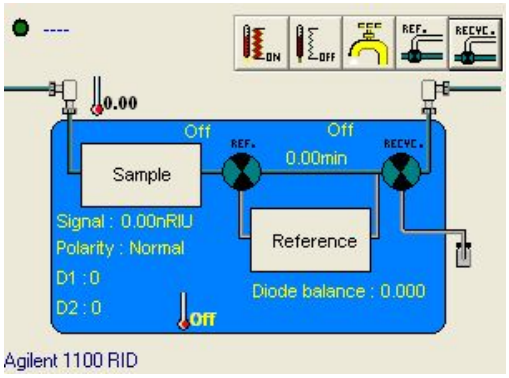
The
button switches on the purge valve.

The

button displays the reference valve control parameters. The available valve positions are: *Sample cell only* and *Reference and sample cells.* This action can be infinite or can begin at a precise time.

The

button displays the recycle valve control parameters. The available valve positions are: *Cell to waste* and *Cell to solvent reservoir.* This action can be infinite or can begin at a precise time.



Not ready: contains the not ready information sent by the instrument.

Events: contains the events that have occurred on the instrument.

Running Instrument Maintenance Software

Software Presentation

Instrument Maintenance Software is a maintenance tool that enables users to perfectly schedule and run the instrument maintenance actions. The Instrument Maintenance Software permits the exchange of components based directly on the intensity if usage and on the analytical conditions.

The Instrument Maintenance Software monitors the usage of components in the instrument. It provides accurate counters and a wear rate that indicates if maintenance procedures should be scheduled or not.

The Instrument Maintenance Software allows tracking the last instrument events

The Instrument Maintenance Software enables users to perform a series of tests functions for troubleshooting and verification. It permits users to also record maintenance actions.

The Instrument Maintenance Software provides also a detailed maintenance audit trail.

Software Functions

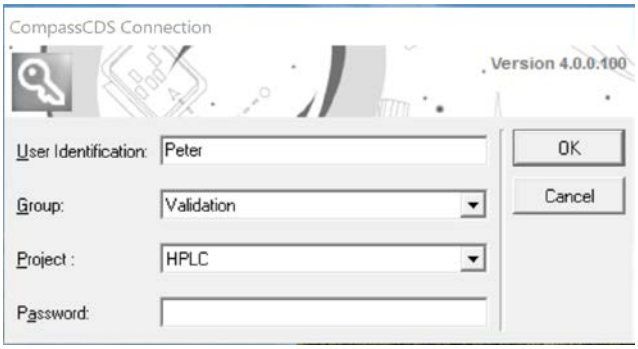
Log in Instrument Maintenance Software

Access the Instrument Maintenance Software in the Client directory of CompassCDS and run it by double-clicking on the executable file (CompassCDS_IMS.exe)

The Instrument Maintenance Software can be run with the CompassCDS version 3.0.2.144 and later.

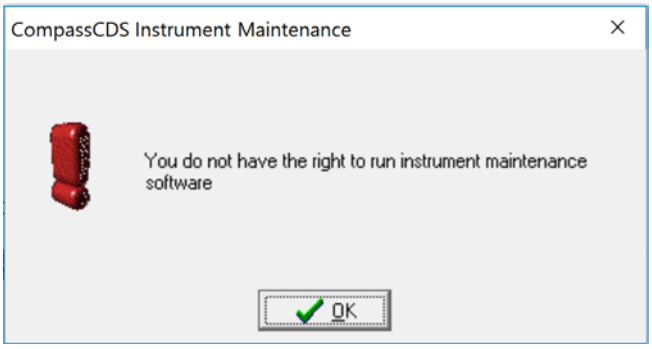
NOTE: the Agilent 1260 Infinity HPLC modules are supported only from CompassCDS 3.0.2.144 and the modules drivers do not support the Instrument Maintenance Software

When the logon window appears, enter a User identification, and choose the group and project in which the system to be maintained is defined in CompassCDS. Type the corresponding password. The password is case sensitive (abc ≠ ABC)



To be able to log into the Instrument Maintenance Software, “allow to run instrument maintenance software” must be checked in the Acquisition/system properties part of the user profile.

If the user does not have the right to run maintenance software, the following message is displayed:



Performing Maintenance and Diagnosis

Run the separate Instrument maintenance software program. Select the system to display the diagnosis screens. It is only possible to display the logbooks and the counters.

You must activate the maintenance mode to be able to modify counters and to perform maintenance and diagnosis actions. Do this by right clicking on the instrument name and selecting *Maintenance On.*

Systems currently in maintenance mode are preceded by the tools symbol:

Diagnostic Section for the Agilent Technologies 1260 Modules

Maintenance of the Agilent Technologies 1260 Autosampler (G1313)

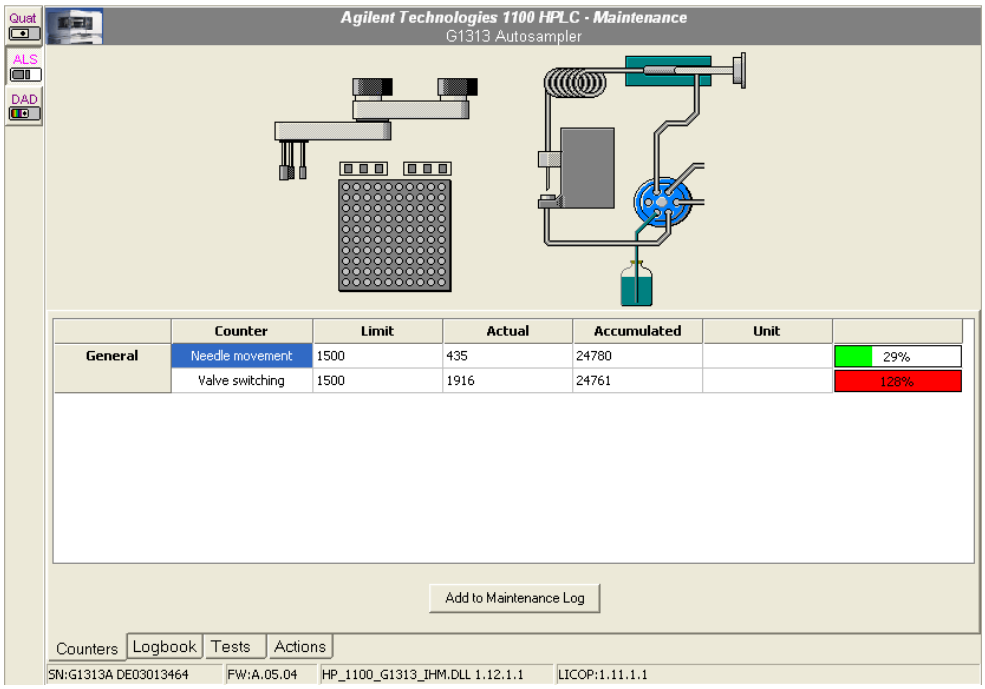
Click on the

button to display the Agilent Technologies 1260 Autosampler (G1313) diagnostic screen. It contains four sub-sections: *Counters, Logbook, Tests* and *Actions*. Click on the required sub-section to display the corresponding screen.

Counters Window

This window permits you to monitor the usage of two components of the autosampler which is schematized at the top of the counters tab.

The counters limits, actual and accumulated values are displayed in the counters table:



The *Limit* values correspond to the maximum allowed values for the counters before the maintenance is needed.

The *Actual* column displays the incremented counter value since the last reset of the counters.

In the *Limit* and *Actual* columns, select the current value and modify it. Validate by pressing the button.

The *Accumulated* values correspond to counter value since the first operation of the autosampler module.

At the right of the table, a visual illustration shows the usage of each counter. Below 75%, the usage is typified in green and above 75% in red to alert that maintenance will be required soon.

Each counter modification is automatically listed in the maintenance audit trail.

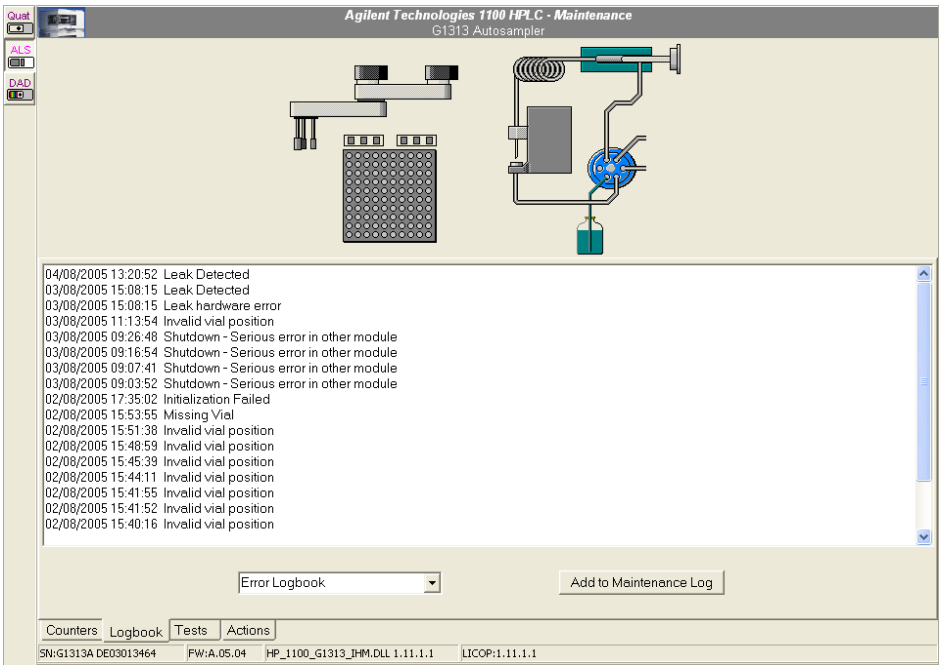
Press Add to Maintenance Log to add the current counters table in the maintenance audit trail.

Counters definition

Needle Movement: Total number of needle movements into the seat.

Valve switching: Total number of injection valve switches.

Logbook Window

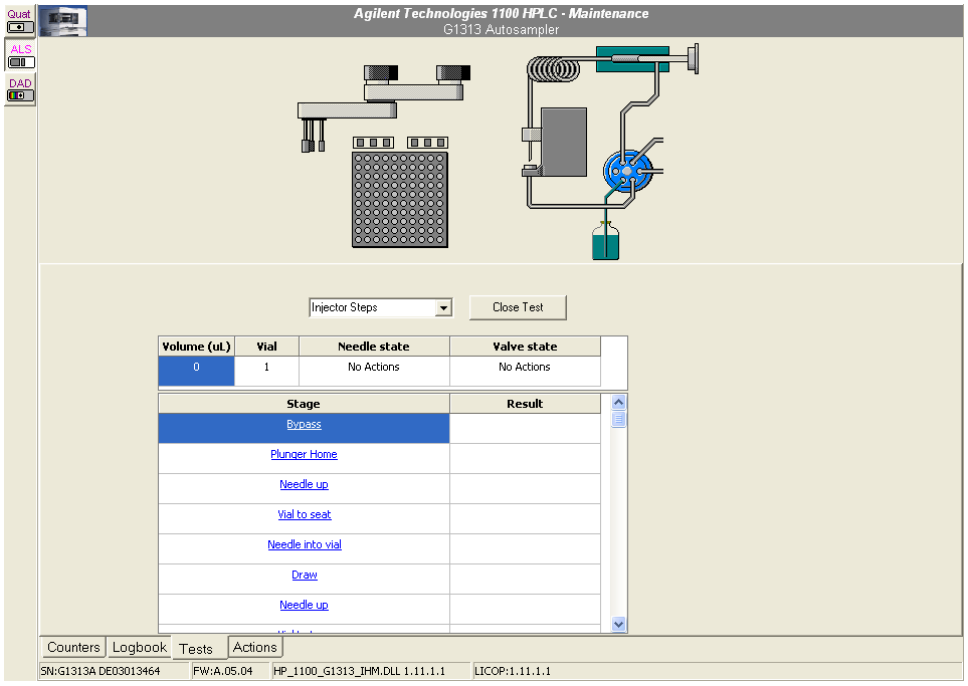


Select a logbook in the scrolling list. The available logbooks are:

- Error logbook
- State change history
- Info event history
- Limit event history
- Error logbook of last analysis
- State change history of last analysis
- Info event history of last analysis
- Limit event history of last analysis
- Parameters changes during the last analysis
- Run history
- Maintenance history

Press to add the displayed logbooks in the maintenance audit trail.

Tests Window



Select a test in the scrolling list. *Injector Steps* and *Gripper Verification* tests are available.

To finish a test, click on the Close Test button. The autosampler is then automatically re-initialized.

Injector steps test

Select *Injector Steps* to check separately the performance of each movement of the injection sequence.

Before performing the tests, enter the required *volume* and *vial* number in the table header.

The following injector test stages are available:

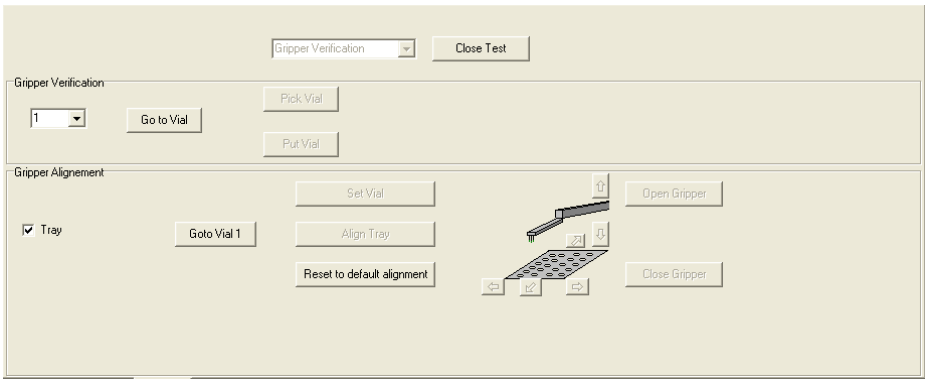
Bypass: switches injection valve to the bypass position.
Plunger home: Moves the plunger to the home position.
Needle up: Lifts the needle arm to the upper position.
Vial to seat: Moves the selected vial to the seat position.
Needle into vial: Lowers the needle into vial.
Draw: Device draws the defined injection volume.
Needle up: Lifts the needle out of the vial.
Vial to tray: Returns the selected vial to the tray position.
Needle into seat: Lowers the needle arm into the seat.
Mainpass: Switches the injection valve to the mainpass position.

Click on a stage to perform it. At the end of a stage, the test result is displayed in the corresponding column and the current needle and valve states are displayed in the table header. Results are also listed in the maintenance audit trail:

It is possible to perform only chosen stages and to perform them several times.

For analyzing the test results, refer to the autosampler operating manual.

Gripper Verification test



Gripper Verification

Run the *Gripper Verification* procedure to verify the gripper alignment is correct.

The test uses 4 vial positions as reference positions. In the scrolling list select the vial for the position check.

Press Go to Vial to move the gripper arm to the vial position.

Press Pick Vial to lift the vial from its position.

Press Put Vial to replace the vial in the tray.

Repeat the procedure for the next vial.

Gripper Alignment

Perform a *Gripper Alignment* procedure if a misalignment is noticed during the *Gripper Verification* test. To correct all other vial positions within the tray, the *Gripper Alignment* procedure uses two vials position as reference points.

Check *Tray* to begin the realignment procedure.

Press Goto Vial 1 to move the gripper arm to position of vial 1.

Press Close Gripper to close the gripper and move the fingers as close as possible to the top of the vial.

Use the arrows keys for correcting rotational, horizontal and vertical position.

Press Open Gripper to open the gripper and move it in such a way that the cap of the vial and rubber of gripper fingers have the same height.

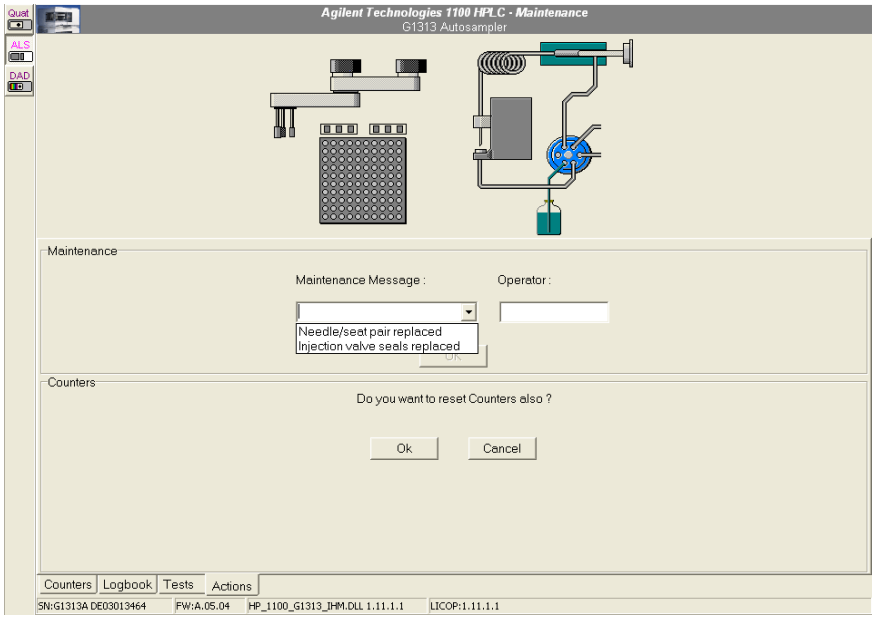
Press Set Vial to validate the new vial 1 position.

Press Goto Vial 81 and repeat the same steps to correct the vial 81 position. Once the vial 81 is aligned, press Set Vial.

Once vial 1 and 81 positions are corrected, press the Align Tray button to realign the tray. The new alignment is stored permanently and the module is reset.

Press Reset to default alignment during the procedure to cancel all correction and set previous alignment.

Actions Window



This window is used to list the autosampler maintenance actions.

Select the replaced component in the *Maintenance Message* scrolling list. Enter the *Operator* name and press the OK button.

The user is then automatically asked if he wants to reset the counters also.

Answer OK to set the corresponding counter actual value to zero or Cancel to not change the actual counter value.

The available choices are *Injection valve seals replaced* and *Needle/seat pair replaced.*

Once an action is performed, it is automatically listed in the maintenance audit trail.

Maintenance of the Agilent Technologies 1260 Quaternary pump (G1311)

Click on the Quat button to display the Agilent Technologies 1260 Quaternary Pump (G1311) diagnostic screen. It contains four sub-sections: *Counters, Logbook, Tests* and *Actions*. Click on the required sub-section to display the corresponding screen.

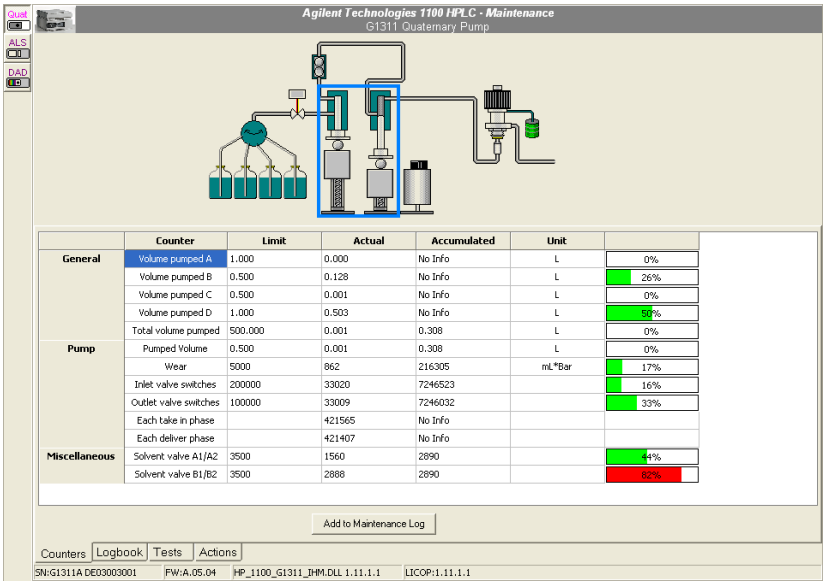
Counters Window

This window monitors the usage of several components of the quaternary pump module which is schematized at the top of the counters tab.

Two different counters tables are available: one for the pump components and another for the valves components. Click on the graphic to select either the pump or valve for display. A box will be highlighted around the displayed component.

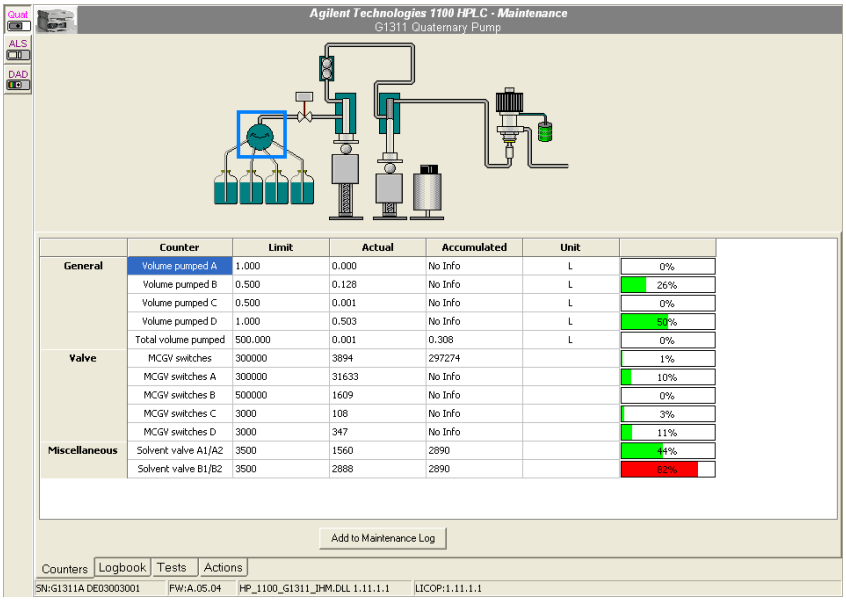
The *General* and *Miscellaneous* counters are identical for the pump and MCGV counters tables. The *Valve* counters are displayed only when selecting the MCGV in the module schema.

Select the pump in the module schema. The following counters limits, actual and accumulated values are displayed and the pump is bordered with a blue rectangle:



	Counter	Limit	Actual	Accumulated	Unit	
General	Volume pumped A	1.000	0.000	No Info	L	0%
	Volume pumped B	0.500	0.128	No Info	L	26%
	Volume pumped C	0.500	0.001	No Info	L	0%
	Volume pumped D	1.000	0.503	No Info	L	50%
	Total volume pumped	500.000	0.001	0.308	L	0%
Pump	Pumped Volume	0.500	0.001	0.308	L	0%
	Wear	5000	862	216305	mL*Bar	17%
	Inlet valve switches	200000	33020	7246523		16%
	Outlet valve switches	100000	33009	7246032		33%
	Each take in phase		421565	No Info		
	Each deliver phase		421407	No Info		
Miscellaneous	Solvent valve A1/A2	3500	1560	2890		44%
	Solvent valve B1/B2	3500	2888	2890		82%

Select the MCGV in the module schema. The following counters limits, actual and accumulated values are then displayed and the MCGV is bordered with a blue rectangle:



	Counter	Limit	Actual	Accumulated	Unit	
General	Volume pumped A	1.000	0.000	No Info	L	0%
	Volume pumped B	0.500	0.128	No Info	L	26%
	Volume pumped C	0.500	0.001	No Info	L	0%
	Volume pumped D	1.000	0.503	No Info	L	50%
	Total volume pumped	500.000	0.001	0.308	L	0%
Valve	MCGV switches	300000	3894	297274		1%
	MCGV switches A	300000	31633	No Info		10%
	MCGV switches B	500000	1609	No Info		0%
	MCGV switches C	3000	108	No Info		3%
	MCGV switches D	3000	347	No Info		11%
Miscellaneous	Solvent valve A1/A2	3500	1560	2890		44%
	Solvent valve B1/B2	3500	2888	2890		82%

The *Limit* values correspond to the maximum allowed values for the counters before the maintenance is needed.

The *Actual* column displays the incremented counter value since the last reset of the counters.

In the *Limit* and *Actual* columns, select the current value and modify it. Validate by pressing the button.

The counter values of the *Volume pumped A to D* cannot be modified. The *Limit* value corresponds to the last fill bottle volume. The *Actual* value is equal to the subtraction of the limit volume by the remaining volume in bottle.

The *Accumulated* values correspond to counter value since the first operation of the pump module.

At the right of the table, a visual illustration shows the usage of each counter. Below 75%, the usage is typified in green and above 75% in red to alert that maintenance will be required soon.

Each counter modification is automatically listed in the maintenance audit trail.

Press

to add the current counters table in the maintenance audit trail.

Counters definition

Volume pumped A: total pumped volume of solvent A.

Volume pumped B: total pumped volume of solvent B.

Volume pumped C: total pumped volume of solvent C.

Volume pumped D: total pumped volume of solvent D.

Total Volume pumped: Sum of the pumped volume of each solvent channel.

Pumped volume: Total pumped volume. It is incremented by the stroke volume with each piston reversal.

Wear: The seal wear value is derived from system pressure and flow, is used as an indicator of seal wear in the pump head. The value increments continually with pump usage.

Inlet valve switches: total number of active-inlet valve switches. The value increments by one with each pump cycle.

Outlet valve switches: total number of outlet-valve switches. The value increments by one with each pump cycle.

Each take in phase: total number of times the plungers reached the take-in phase state.

Each deliver phase: total number of times the plungers reached the delivery phase state.

Solvent valve A1/A2: Total number of solvent selection valve A switches.

Solvent valve B1/B2: Total number of solvent selection valve B switches.

MCGV switches: Total number of interrupts for MCGV switches.

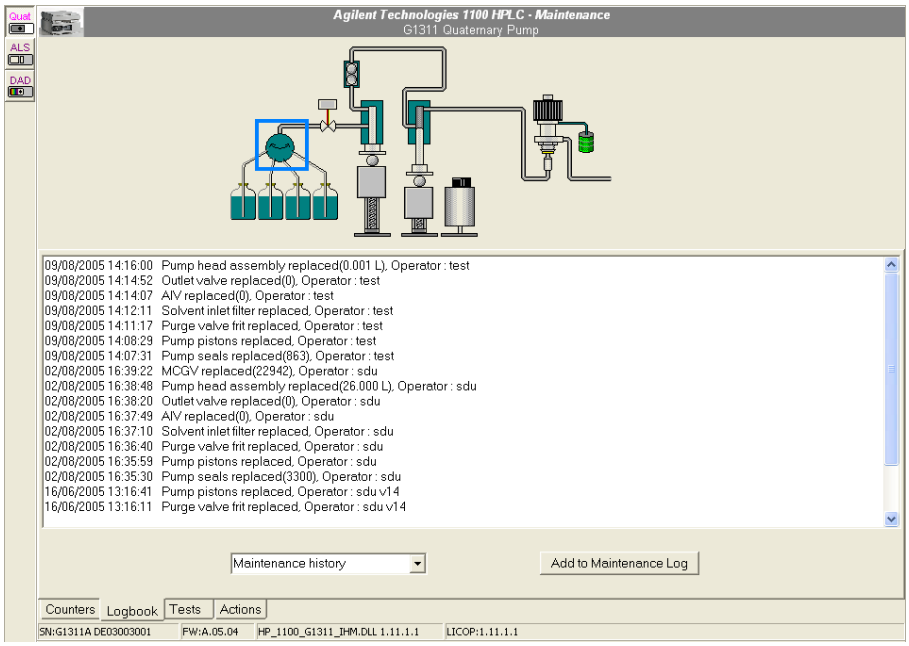
MCGV switches A: Total number of channel A valve switches.

MCGV switches B: Total number of channel B valve switches.

MCGV switches C: Total number of channel C valve switches.

MCGV switches D: Total number of channel D valve switches.

Logbook Window


Agilent Technologies 1100 HPLC - Maintenance
G1311 Quaternary Pump
Quat
ALS
DAD
09/08/2005 14:16:00 Pump head assembly replaced(0.001 L), Operator : test
09/08/2005 14:14:52 Outlet valve replaced(0), Operator : test
09/08/2005 14:14:07 AIV replaced(0), Operator : test
09/08/2005 14:12:11 Solvent inlet filter replaced, Operator : test
09/08/2005 14:11:17 Purge valve frit replaced, Operator : test
09/08/2005 14:08:29 Pump pistons replaced, Operator : test
09/08/2005 14:07:31 Pump seals replaced(863), Operator : test
02/08/2005 16:39:22 MCGV replaced(22942), Operator : sdu
02/08/2005 16:38:48 Pump head assembly replaced(26.000 L), Operator : sdu
02/08/2005 16:38:20 Outlet valve replaced(0), Operator : sdu
02/08/2005 16:37:49 AIV replaced(0), Operator : sdu
02/08/2005 16:37:10 Solvent inlet filter replaced, Operator : sdu
02/08/2005 16:36:40 Purge valve frit replaced, Operator : sdu
02/08/2005 16:35:59 Pump pistons replaced, Operator : sdu
02/08/2005 16:35:30 Pump seals replaced(3300), Operator : sdu
16/06/2005 13:16:41 Pump pistons replaced, Operator : sdu v14
16/06/2005 13:16:11 Purge valve frit replaced, Operator : sdu v14
Maintenance history
Add to Maintenance Log
Counters
Logbook
Tests
Actions
SN:G1311A DE03003001
FW:A.05.04
HP_1100_G1311_IHM.DLL 1.11.1.1
LICOP:1.11.1.1

Select in the scrolling list the logbook to display. The available logbooks are:

Error logbook
State change history
Info event history
Limit event history
Error logbook of last analysis
State change history of last analysis
Info event history of last analysis
Limit event history of last analysis
Parameters changes during the last analysis
Run history
Maintenance history

Press Add to Maintenance Log to add the displayed logbook in the maintenance audit trail.

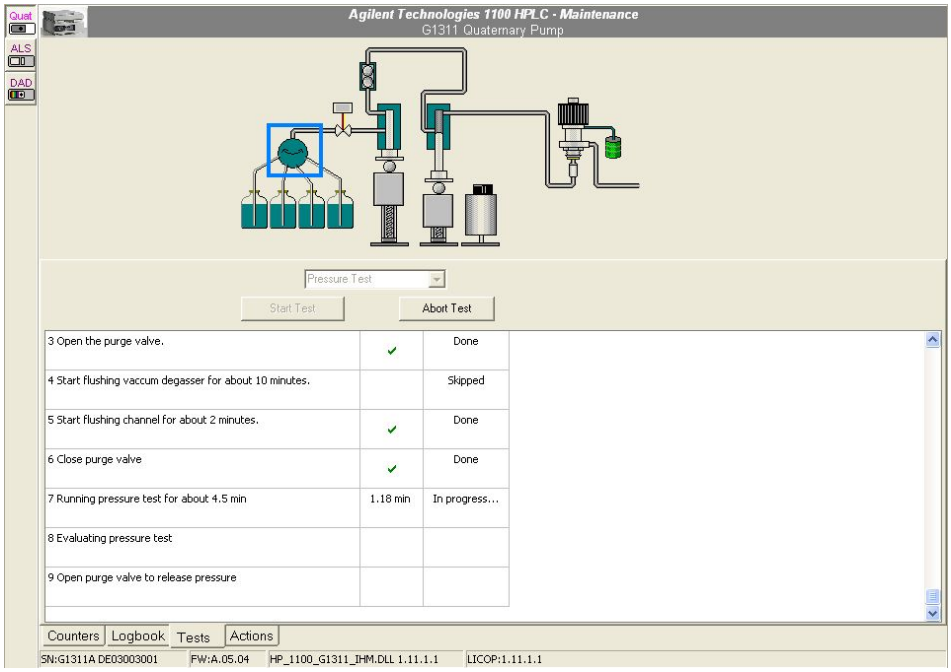
Tests Window

Select a test in the scrolling list and press Start Test to start the test. *Pressure Test* and *Leak Test* are available.

Follow the instructions and once a stage is done, press *Continue* or *Skip* in the status column.

It is possible to stop the test at any one stage by pressing the Abort Test button.

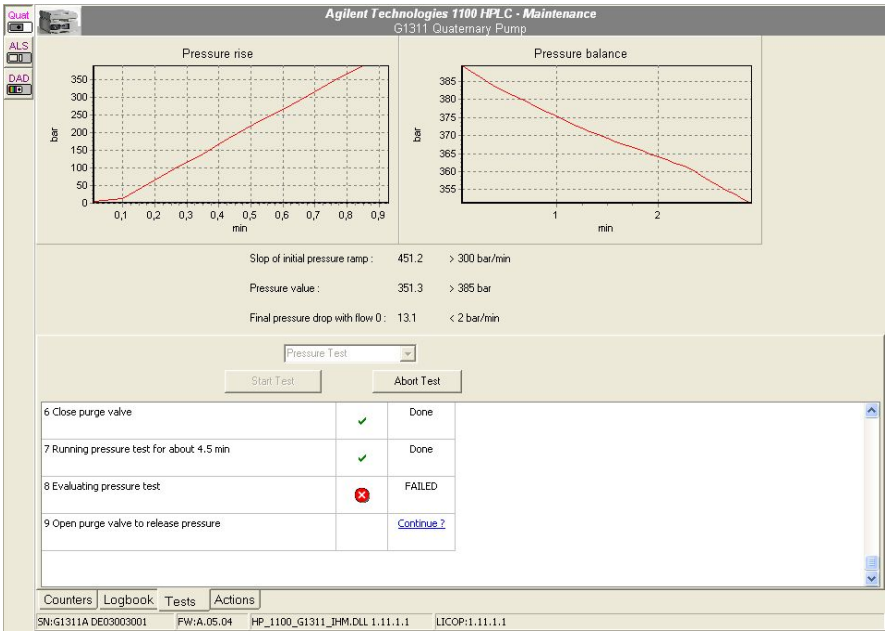
Pressure test


Agilent Technologies 1100 HPLC - Maintenance
G1311 Quaternary Pump
Quat
ALS
DAD
Pressure Test
Start Test
Abort Test
3 Open the purge valve. Done
4 Start flushing vaccum degasser for about 10 minutes. Skipped
5 Start flushing channel for about 2 minutes. Done
6 Close purge valve Done
7 Running pressure test for about 4.5 min 1.18 min In progress...
8 Evaluating pressure test
9 Open purge valve to release pressure
Counters Logbook Tests Actions
SN:G1311A DE03003001 FW:A.05.04 HP_1100_G1311_IHM.DLL 1.11.1.1 LICOP:1.11.1.1

Perform the *Pressure Test* to demonstrate pressure–tightness up to 400 bars. The test consists in monitoring pressure profile while the pump is following defined stages.

After its initialization, the pump starts pumping isopropyl alcohol with a flow rate of 510µL/min and a stroke of 100 µL. When the system pressure reaches the 390s bar value, the pump switches off.

Once the pressure test is finished, results are displayed on screen and also in the maintenance audit trail:

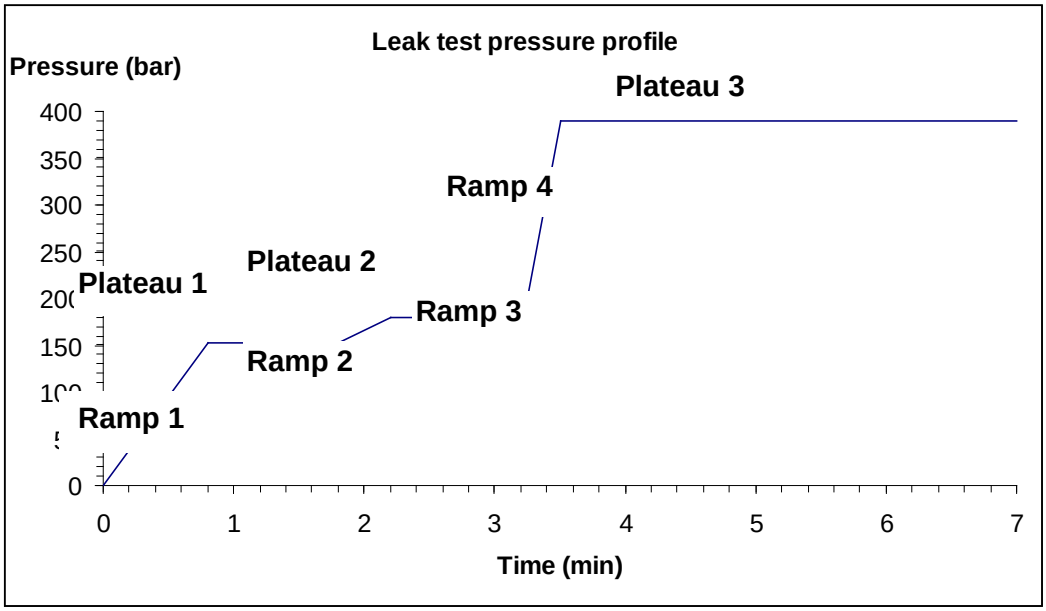

Agilent Technologies 1100 HPLC - Maintenance
G1311 Quaternary Pump
Quat
ALS
DAD
Pressure rise
Pressure balance
bar
min
Slop of initial pressure ramp : 451.2 > 300 bar/min
Pressure value : 351.3 > 385 bar
Final pressure drop with flow 0 : 13.1 < 2 bar/min
Pressure Test
Start Test
Abort Test
6 Close purge valve Done
7 Running pressure test for about 4.5 min Done
8 Evaluating pressure test FAILED
9 Open purge valve to release pressure Continue ?
Counters Logbook Tests Actions
SN:G1311A DE03003001 FW:A.05.04 HP_1100_G1311_IHM.DLL 1.11.1.1 LICOP:1.11.1.1

For analyzing the test results, refer to the pump operating manual.

Leak test

Run the *Leak Test* if the pump is the source of the leak.

The test consists in monitoring pressure profile while the pump is following defined stages, different from those of the pressure test:



Ramp 1: The pump is initialized and then plunger 1 delivers a 153 µL/min flow of isopropyl alcohol with a stroke length of 100 µL.

Plateau 1: Plunger 2 delivers a 2µL/min flow rate during 1 minute.

Ramp 2: Plunger 2 delivers a 153 µL/min flow and plunger 1 pumps to complete the second half of the ramp.

Plateau 2: Plunger 1 delivers a 2 µL/min flow for 1 minute.

Ramp 3: The stroke is changed to 100 µL and the flow is increased to 220 µL/min and then to 510 µL/min.

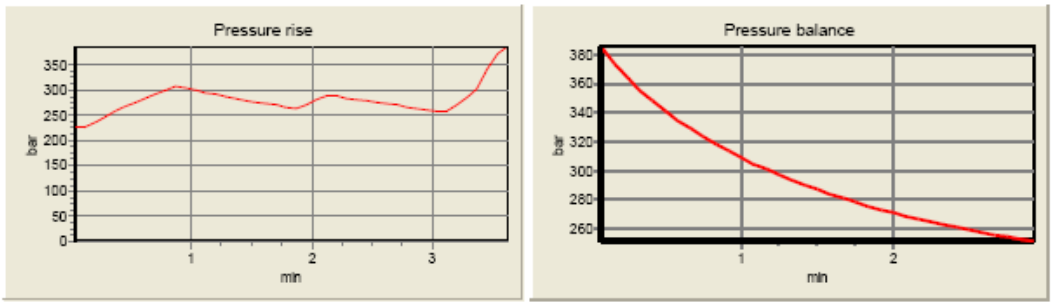
Ramp 4: The system reaches 390 bars and the flow is stopped.

Plateau 3: The pressure drop should not exceed 2 bars/min.

The pressure should stay constant during the plateau and should increase linearly during the ramps.

Once the leak test is finished, results are displayed on screen and also in the maintenance audit trail:

Leak Test performed the 03/08/2005 at 10:04:18

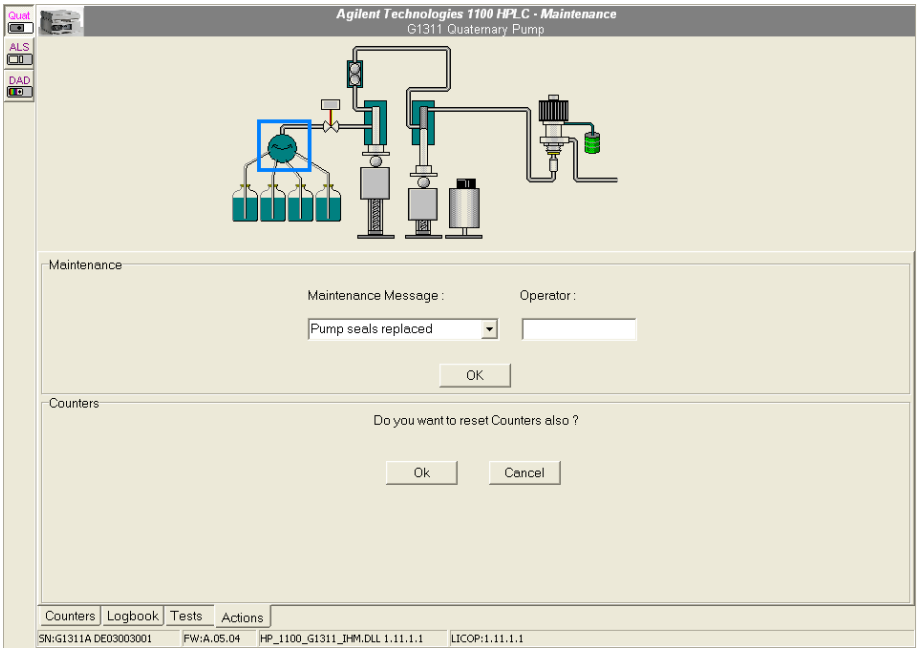


Test Result :

Test	Test values	Test limits	Test results
Pressure for the first plateau :	267.0	> 100 bar	Passed
Slope of the first plateau :	52.9	> 0 bar/min	Passed
Pressure for the second plateau :	259.1	> 140 bar	Passed
Slope for the second plateau :	65.4	> 0 bar/min	Passed
Pressure value :	249.4	> 385 bar	Failed
Final pressure drop with flow 0 :	46.7	< 2 bar/min	Failed

For analyzing the test results, refer to the pump operating manual.

Actions Window



This window is used to list the pump module maintenance actions.

Select the replaced component in the *Maintenance Message* scrolling list. Enter the *Operator* name and press the OK button.

The user is then automatically asked if he wants to reset the corresponding counters also.

Answer OK to set the corresponding counter actual value to zero or Cancel to not change the actual counter value.

The available choices are:

Pump seals replaced: Actual Wear and Pumped volume counters can be reset.

Pump pistons replaced: no outcome on counters.

Purge valve frit replaced: no outcome on counters

Solvent inlet filter replaced: no outcome on counters

AIV (Active Inlet Valve): Actual Inlet valve switches counters can be reset.

Outlet valve: Actual Inlet valve switches counters can be reset.

Pump head assembly: no outcome on counters

MCGV (Multi Channel gradient Valve) replaced: MCGV switches counters from A to D can be reset.

Once an action is performed, it is automatically listed in the maintenance audit trail.

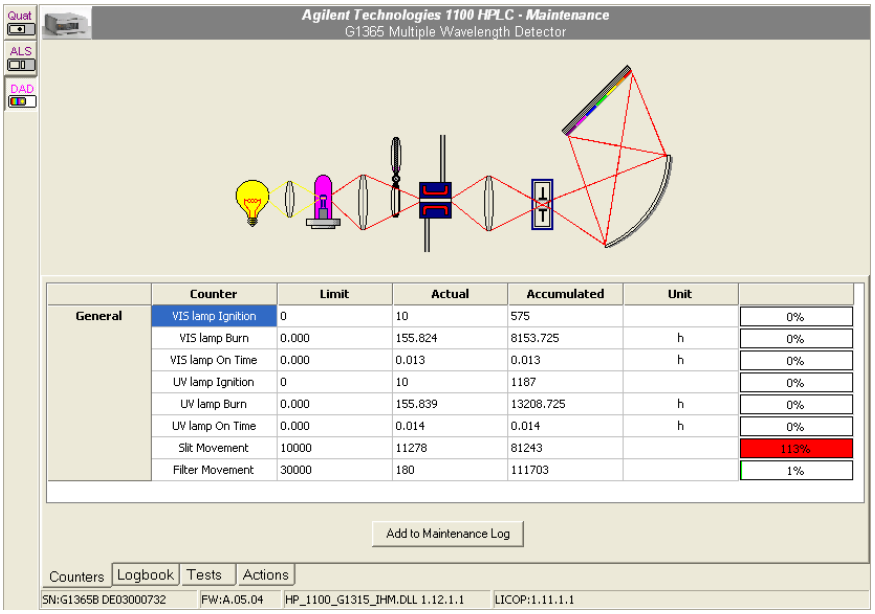
Maintenance of the Agilent Technologies 1260 Diode Array Detector (G1315) and Multiple Wavelength Detector (G1365)

Click on the DAD button to display the Agilent Technologies 1260 Diode Array Detector (G1315) and Multiple Wavelength detector (G1365) diagnostic screen. It contains four sub-sections: *Counters, Logbook, Tests* and *Actions*. Click on the required sub-section to display the corresponding screen.

Counters Window

This window monitors the usage of several components of the detector module which is schematized at the top of the counters tab.

The following counter limits, actual and accumulated values are then displayed:



	Counter	Limit	Actual	Accumulated	Unit	
General	VIS lamp Ignition	0	10	575		0%
	VIS lamp Burn	0.000	155.824	8153.725	h	0%
	VIS lamp On Time	0.000	0.013	0.013	h	0%
	UV lamp Ignition	0	10	1187		0%
	UV lamp Burn	0.000	155.839	13208.725	h	0%
	UV lamp On Time	0.000	0.014	0.014	h	0%
	Slit Movement	10000	11278	81243		113%
	Filter Movement	30000	180	111703		1%

The *Limit* values correspond to the maximum allowed values for the counters before the maintenance is needed.

The *Actual* column displays the incremented counter value since the last reset of the counters.

In the *Limit* and *Actual* columns, select the current value and modify it. Validate by pressing the button.

The counter values of the *VIS lamp Ignition*, VIS lamp Burn, *UV lamp Ignition* and *UV lamp Burn* cannot be modified. The A*ctual* values are respectively equal to the *Lamp Ignition* and *Lamp On-Time* values displayed in the detector status.

The *Accumulated* values correspond to counter value since the first operation of the pump module.

At the right of the table, a visual illustration shows the usage of each counter. Below 75%, the usage is typified in green and above 75% in red to alert that maintenance will be required soon.

Each counter modification is automatically listed in the maintenance audit trail.

Press Add to Maintenance Log to add the current counters table in the maintenance audit trail.

Counters definition

VIS/UV Lamp Ignition: number of ignition of the lamps.

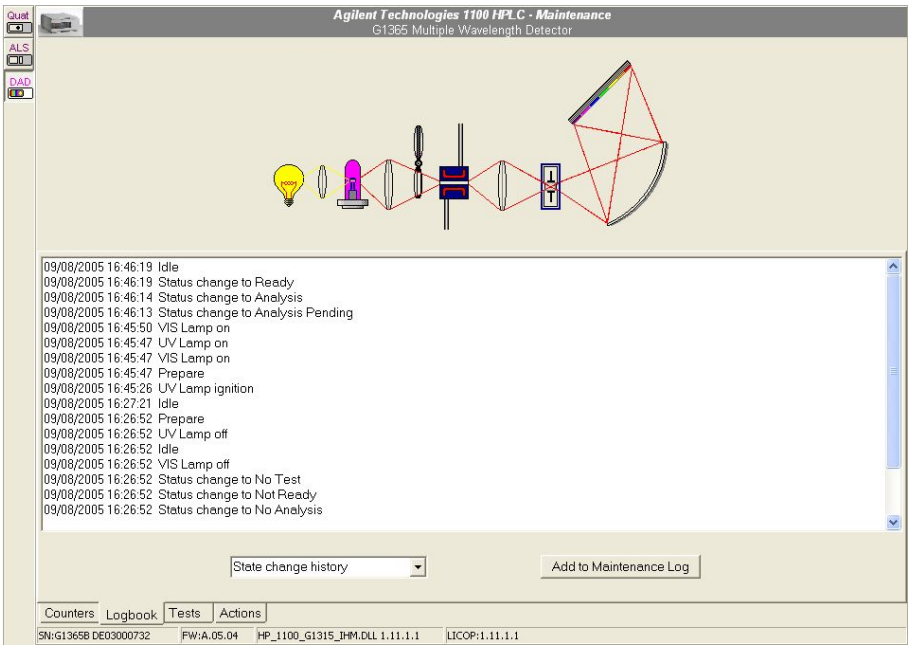
VIS/UV Lamp Burn: Tungsten/deuterium lamp total burn time.

VIS/UV Lamp On-time: Tungsten/deuterium lamp burn time since the last ignition.

Slit Movement: Number of movements of the slit assembly.

Filter Movement: Number of movements of the filter assembly.

Logbook Window



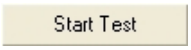
Select in the scrolling list the logbook to display. The available logbooks are:

Error logbook
State change history
Info event history
Limit event history
Error logbook of last analysis
State change history of last analysis
Info event history of last analysis
Limit event history of last analysis
Parameters changes during the last analysis
Run history
Maintenance history

Press

to add the displayed logbook in the maintenance audit trail.

Tests Window

Select a test in the scrolling list and press 

to start the test. The available tests are:

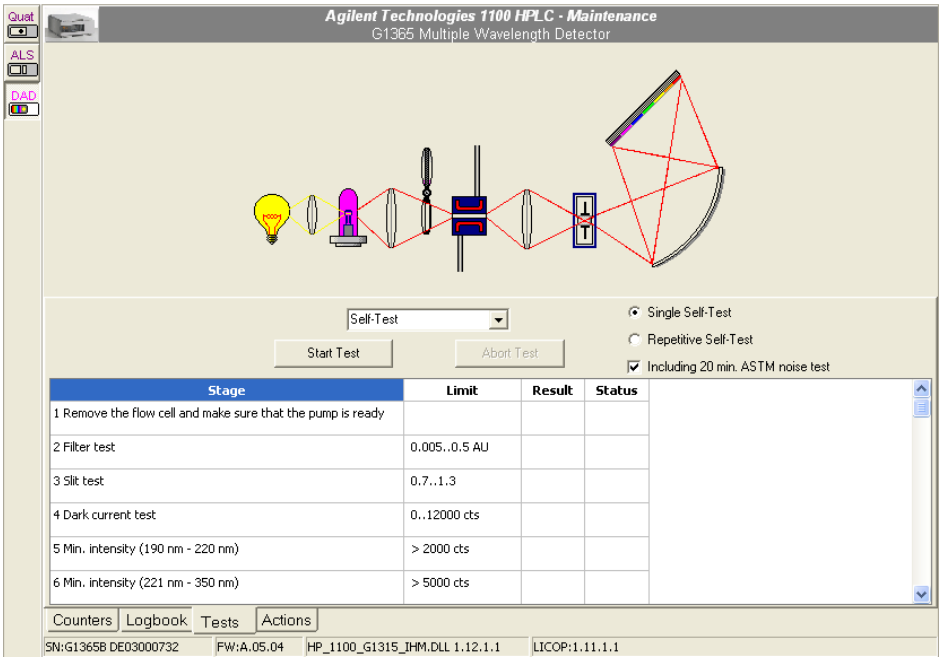
Self-Test
Dark Current Test
Intensity Test
Holmium Test
Cell Test
Filter Test
WL. Calibration Test
D/A Converter Test

Follow the instructions and once a stage is done, press *Continue* or *Skip* in the status column.

It is possible to stop the test at any one stage by pressing the

button.

Self-Test Test



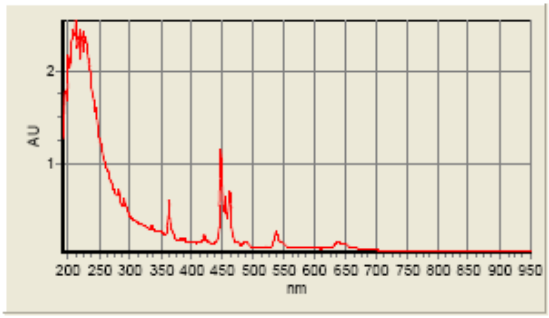
The *Self-Test* test consists in running the following individual tests consecutively: Filter Test, Slit Test, Dark Current Test, Wavelength Calibration test, Intensity test, Holmium Test, spectral flatness test and ASTM noise test if checked before starting the Self-test.

Select *Single Self-test* or *Repetitive Self-Test* to run the test once or repetitively. Note that if one of the tests fails for the first cycle, the second cycle will not be started.

The ASTM noise test determines the detector baseline noise (at 254 nm). It must be performed while pumping water at 1 mL/min.

Results are displayed at screen and also in the maintenance audit trail:

Self Test performed the 02/08/2005 at 09:57:52



Test Table :

Stage	Limit	Result	Status
1 Remove the flow cell and make sure that the pump is ready			Done
2 Filter test	0.005..0.5 AU	0.187	Passed
3 Slit test	0.7..1.3	0.909	Passed
4 Dark current test	0..12000 cts	2791..3237cts	Passed
5 Min. intensity (190 nm - 220 nm)	> 2000 cts	1186	Failed
6 Min. intensity (221 nm - 350 nm)	> 5000 cts	10251	Passed
7 Min. intensity (351 nm - 500 nm)	> 2000 cts	8453	Passed
8 Min. intensity (501 nm - 950 nm)	> 4000 cts	23139	Passed
9 Max. intensity (190 nm - 350 nm)	< 450000 cts	30359	Passed
10 Max. intensity (700 nm - 950 nm)	< 300000 cts	89020	Passed
11 Max. intensity (D2 alpha line)	< 1200000 cts	169581	Passed
12 Wavelength at 486.0 nm	485.5..486.5 nm	486.00	Passed
13 Wavelength at 656.1 nm	655.6..656.6 nm	656.09	Passed
14 Holmium test	-1..1 nm	-2.22	Failed
15 Spectral flatness	< 0.002 AU	0.0001	Passed

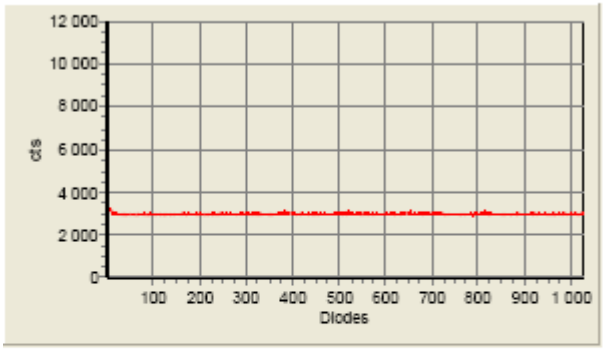
For analyzing the test results, refer to the detector operating manual.

Dark Current Test

Perform the *Dark Current* test to determine the leakage current from each optical diode. This leakage current may cause non-linearity or excessive noise at specific wavelengths.

When starting the test, the 1 nm slit assembly is moved to the dark position. At the end of the dark current test, the resulting leakage current is measured and graphically displayed for each diode. Results are also listed in the maintenance audit trail:

Dark Test performed the 02/08/2005 at 10:01:44



Test Table :

Stage	Limit	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.			Done
2 Dark current maximum value	<= 12000 cts	3284cts	Passed
3 Dark current minimum value	> 0 cts	2817cts	Passed

For analyzing the test results, refer to the detector operating manual.

Intensity Test

Perform the *Intensity* test to evaluate the performance of the lamps and optics. UV and VIS lamps Intensity are measured over the detector wavelengths range.

The test should be done with water in the flow cell.

When starting the test, the 1 nm slit is moved into the light path and the gain is set to zero. Four spectral ranges are used to evaluate the intensity spectrum. Results are displayed on screen and also listed in the maintenance audit trail:

Intensity Test performed the 02/08/2005 at 10:02:16

Test Table :

Stage	Limit	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.			Done
2 Min. intensity (190 nm - 220 nm)	> 2000 cts	1186	Failed
3 Min. intensity (221 nm - 350 nm)	> 5000 cts	10251	Passed
4 Min. intensity (351 nm - 500 nm)	> 2000 cts	8453	Passed
5 Min. intensity (501 nm - 950 nm)	> 4000 cts	23139	Passed
6 Max. intensity (190 nm - 350 nm)	< 450000 cts	30359	Passed
7 Max. intensity (700 nm - 950 nm)	< 300000 cts	89020	Passed
8 Max. intensity (D2 alpha line)	< 1200000 cts	169581	Passed

For analyzing the test results, refer to the detector operating manual.

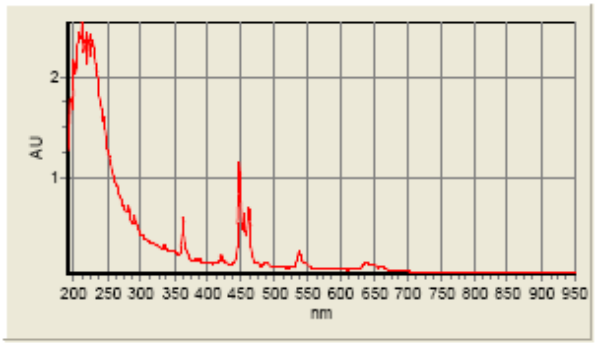
Holmium Test

Perform the *Holmium* test to verify wavelength accuracy. Three characteristic absorbance maxima of the holmium oxide filter are measured.

The test should be done with water in the flow cell.

When starting the test, the 1 nm slit is moved into the light path. Measured maxima are displayed on screen and also listed in the maintenance audit trail:

Holmium Test performed the 02/08/2005 at 10:11:35



Test Table :

Stage	Limit	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.			Done
2 Wavelength 1 (361 nm)	360..362 nm	363.2	Failed
3 Wavelength 2 (453.7 nm)	452.7..454.7 nm	454.9	Failed
4 Wavelength 3 (536.7 nm)	535.7..537.7 nm	537.4	Passed

For analyzing the test results, refer to the detector operating manual.

Cell Test

Perform the *Cell* test to check whether the flow cell window is clean.

The deuterium and tungsten lamps intensity is measured over the detector wavelength range with the flow cell installed and with the flow cell removed.

The test should be done with water in the flow cell.

When starting the test, the 1 nm slit is moved into the light path and the gain is set to zero. The resulting intensity ratio represents the amount of light absorbed by the flow cell. It is displayed at screen and also listed in the maintenance audit trail:

Cell Test performed the 02/08/2005 at 10:15:01

Test Table :

Stage	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.		Done
2 if cell not in place, install it		Done
3 Mesuring intensity with cell	44632	Done
4 Remove cell		Done
5 Mesuring intensity without cell	25615	Done
6 Calculating intensity ratio	1.74	Done

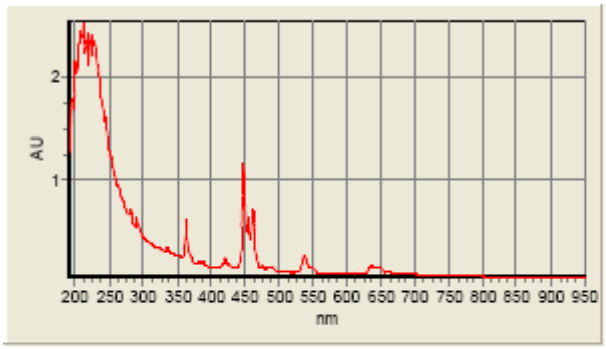
For analyzing the test results, refer to the detector operating manual.

Filter Test

Perform the *Filter* test to determine the if the filter is clean. During the test, the filter motor is moved in specific positions and the resulting absorbance of the holmium oxide filter is monitored.

During the filter movement, the absorbance maxima are measured and then graphically displayed at screen and in the maintenance audit trail:

Filter Test performed the 02/08/2005 at 10:17:40



Test Table :

Stage	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.		Done
2 Mesuring and evaluating filter test result	0.177	Passed

For analyzing the test results, refer to the detector operating manual.

Wavelength Calibration Test

Perform the *Wavelength Calibration* test to check wavelength calibration.

During the test, the alpha (656.1 nm) and beta (486 nm) emission lines deviation of the deuterium lamp are evaluated.

The test should be done with water in the flow cell.

The 1 nm slit is moved into the light path and the gain is set to zero. The largest emission lines deviation is displayed.

At stage 6, choose to use this result to recalibrate the detector by clicking *Yes*. If the deviation is small, click on *No* to ignore the results.

At the end of the re-calibration, the largest emission lines deviation is evaluated again and displayed on screen and also in the maintenance audit trail:

Calibration Test performed the 02/08/2005 at 10:23:24

Test Table :

Stage	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.		Done
2 Remove MWD flow cell		Done
3 Mesuring WL for beta-line (at 486.0 nm)	486.03	Done
4 Mesuring WL for alpha-line (at 656.1 nm)	656.10	Done
5 Evaluating largest deviation from center WL (nm)	0.03	Done
6 Do you want to recalibrate your detector ?		Done
7 Mesuring WL for beta-line (at 486.0 nm)	486.01	Done
8 Mesuring WL for alpha-line (at 656.1 nm)	656.10	Done
9 Evaluating largest deviation from center WL (nm)	0.01	Done

For analyzing the test results, refer to the detector operating manual.

D/A Converter Test

Perform the *D/A Converter* test to check correct operation of the digital-analog-converter.

During the test, a theoretical analog signal of approximately 52 mV with a square wave of 10µV and a frequency of 1 cycle / 48 seconds is applied to the digital-analog-converter (DAC).

The DAC signal must be plotted on an integrator at least 5 minutes in order to measure the amplitude and the peak-to-peak noise of the signal. The results are not directly provided by the Instrument Maintenance Software but by the integrator.

The following performed stages are displayed on screen and also in the maintenance audit trail:

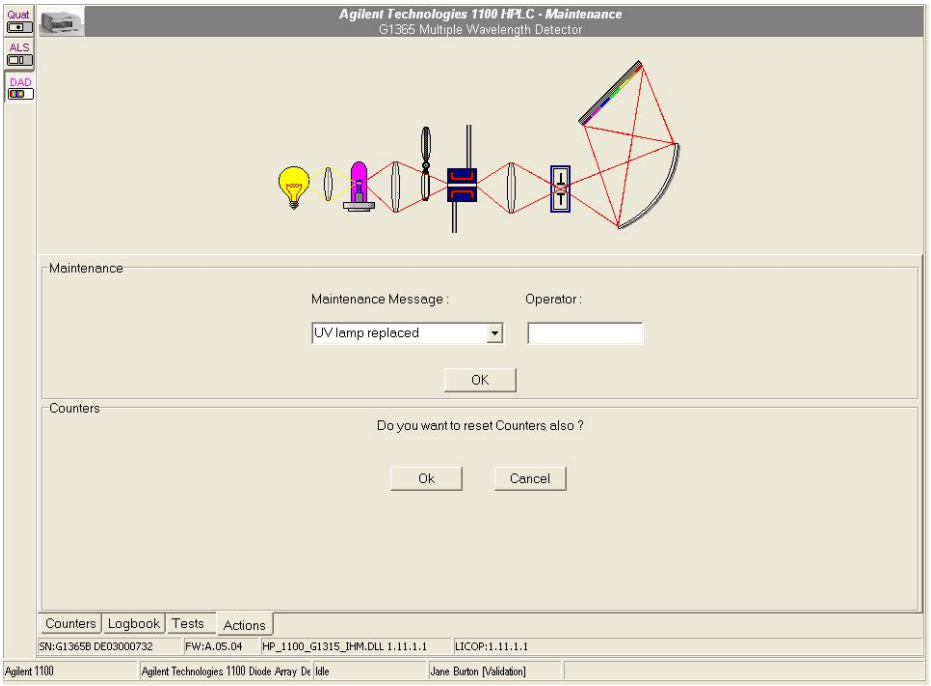
Converter Test performed the 10/08/2005 at 14:41:52

Test Table :

Stage	Result	Status
1 Ensure that the flow cell has non absorbing solvent flowing.		Done
2 Switch test signal to analog output	Test signal available	Done
3 Remove test signal from analog output	Test signal removed	Done

For analyzing the test results, refer to the detector operating manual.

Actions Window



This window is used to list the detector module maintenance actions.

Select the replaced component in the *Maintenance Message* scrolling list. Enter the *Operator* name and press the OK button.

The user is then automatically asked if he wants to reset the counters also.

Answer OK to set the corresponding counter actual value to zero or Cancel to not change the actual counter value.

The available choices are:

UV lamp replaced: UV lamp ignition, UV lamp Burn and UV lamp On Time counters can be reset.
VIS lamp replaced: Vis lamp ignition, Vis lamp Burn and Vis lamp On Time counters can be reset.
Filter assembly replaced: Filter movement counter can be reset.
Optical unit replaced: no outcome on counters
Once an action is performed, it is automatically listed in the maintenance audit trail.

Reporting Maintenance Audit trail

Creating a Maintenance Audit Trail

The maintenance audit trail lists each counter modification, test and maintenance actions performed during the maintenance period. Depending on the module, certain tables can also be added to the maintenance audit trail report.

It is possible to preview, print, save as and open current and existing maintenance audit trails.

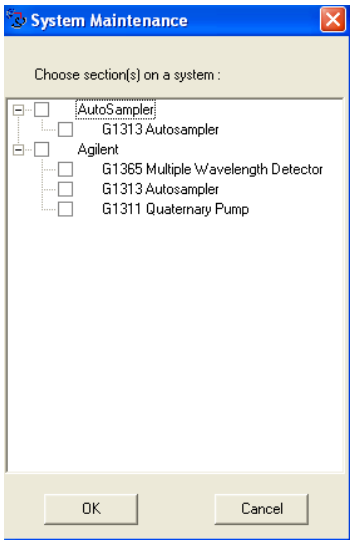
An audit trail maintenance report is automatically created when the maintenance mode is activated. When the maintenance is stopped, it is automatically saved and archived as a PDF file. The automatically generated name follows the template: “system name”_”date”_”time”.pdf. The maintenance audit trail reports are stored on the CompassCDS main server, in the CompassCDS\server\DataShared\Maintenance\”system name” directory.

The maintenance actions are not listed if the maintenance mode is not stopped normally.

Viewing Current Audit Trail

When in maintenance mode, select the ***FILE /AUDIT TRAIL PREVIEW*** menu options, press or right-click on the selected system and choose *Audit Trail Preview* to display the current audit trail. It lists all performed maintenance actions since the system is in maintenance mode for all systems in maintenance mode.

The *System Maintenance* screen is displayed, enabling to choose the systems and modules to display the maintenance audit trail report:



Check the modules to display only the corresponding maintenance audit trail in the report. Check the systems names to display all the maintenance audit trails in the report.

It is possible to zoom in, zoom out and print the report from the preview.

Printing Current Audit Trail

When in maintenance mode, select the ***FILE /PRINT AUDIT TRAIL*** menu options or press to print the current audit trail. It lists all performed maintenance actions since the system is in maintenance mode for all systems in maintenance mode.

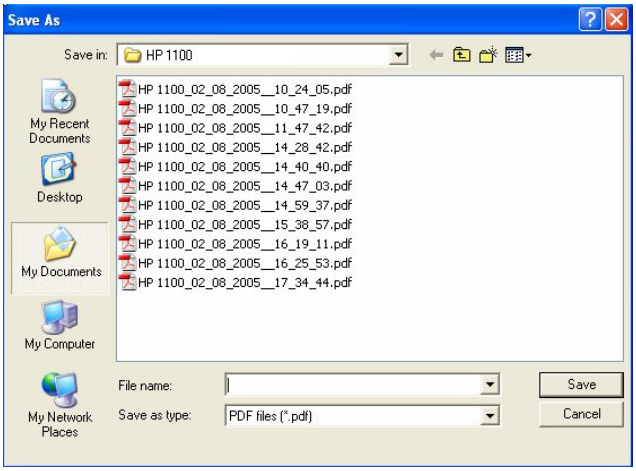
As for the *Audit Trail Preview* function, the *System Maintenance* screen is displayed. Check the required modules and/or systems to print only the corresponding maintenance audit trail in the report.

Saving Current Maintenance Audit Trail

When in maintenance mode, select the ***FILE /SAVE AUDIT TRAIL AS*** menu options or press to save the current maintenance audit trail before the maintenance is stopped.

As for the *Audit Trail Preview* function, the *System Maintenance* screen is displayed. Check the required modules and/or systems to save only the corresponding maintenance audit trail in a report.

Then, choose the storing directory and the file name for the saved maintenance audit trail report:

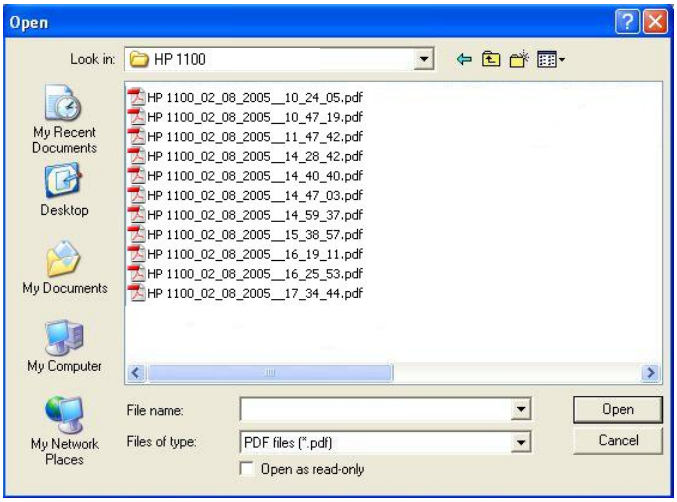


When performing maintenance actions from a station different from the main server, it is advisable to use the *Save As* function. Indeed, saving the audit trail reports on a local path will enable users to easily open existing maintenance audit trail reports later. It is not possible to open automatically generated reports from a station different from the main server because CompassCDS\server\DataShared\Maintenance\ directory is not shared.

Opening a Maintenance Audit Trail

Select the ***FILE /OPEN AUDIT TRAIL*** menu options or press to open an existing maintenance audit trail.

The following screen is open and enables to explore and choose the directory and the maintenance audit trail report to open:



NOTE: When opening reports from the main server, the CompassCDS\server\DataShared\Maintenance\ directory is selected by default. Then, open the system name directory and choose the report to open.

Appendix

GPIB Addresses

The Agilent Technologies 1260-LC Master module connected to CompassCDS with the GPIB cable must have a unique address between 0 and 31. Usually ‘21’ is reserved for IEEE488 controller (GPIB card or *MIB-interface* with GPIB card).

The address is set with an 8 bit switch located on the rear panel of modules. Changing the position of these switches must be done with module switched-off.

The following table shows the switch positions for each GPIB address:

Address	Sw4	Sw5	Sw6	Sw7	Sw8
0	Down	Down	Down	Down	Down
1	Down	Down	Down	Down	Up
2	Down	Down	Down	Up	Down
3	Down	Down	Down	Up	Up
4	Down	Down	Up	Down	Down
5	Down	Down	Up	Down	Up
6	Down	Down	Up	Up	Down
7	Down	Down	Up	Up	Up
8	Down	Up	Down	Down	Down
9	Down	Up	Down	Down	Up
10	Down	Up	Down	Up	Down
11	Down	Up	Down	Up	Up
12	Down	Up	Up	Down	Down
13	Down	Up	Up	Down	Up
14	Down	Up	Up	Up	Down
15	Down	Up	Up	Up	Up
16	Up	Down	Down	Down	Down
17	Up	Down	Down	Down	Up
18	Up	Down	Down	Up	Down
19	Up	Down	Down	Up	Up

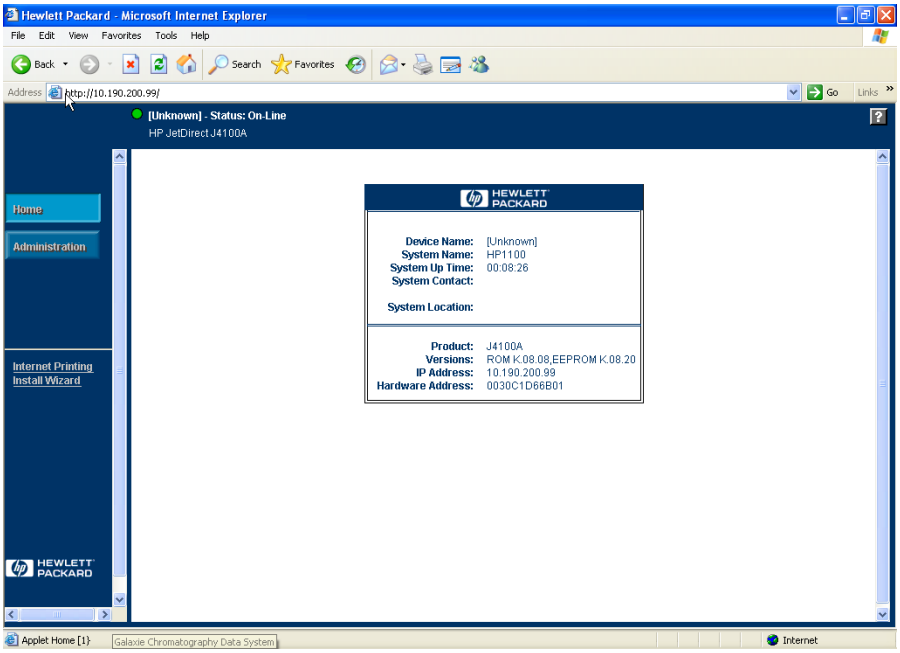
20	Up	Down	Up	Down	Down
21	Up	Down	Up	Down	Up
22	Up	Down	Up	Up	Down
23	Up	Down	Up	Up	Up
24	Up	Up	Down	Down	Down
25	Up	Up	Down	Down	Up
26	Up	Up	Down	Up	Down
27	Up	Up	Down	Up	Up
28	Up	Up	Up	Down	Down
29	Up	Up	Up	Down	Up
30	Up	Up	Up	Up	Down
31	Up	Up	Up	Up	Up

Configuring a Fixed IP Address

This appendix describes how to fix the IP address in the Agilent Technologies 1260 LC.

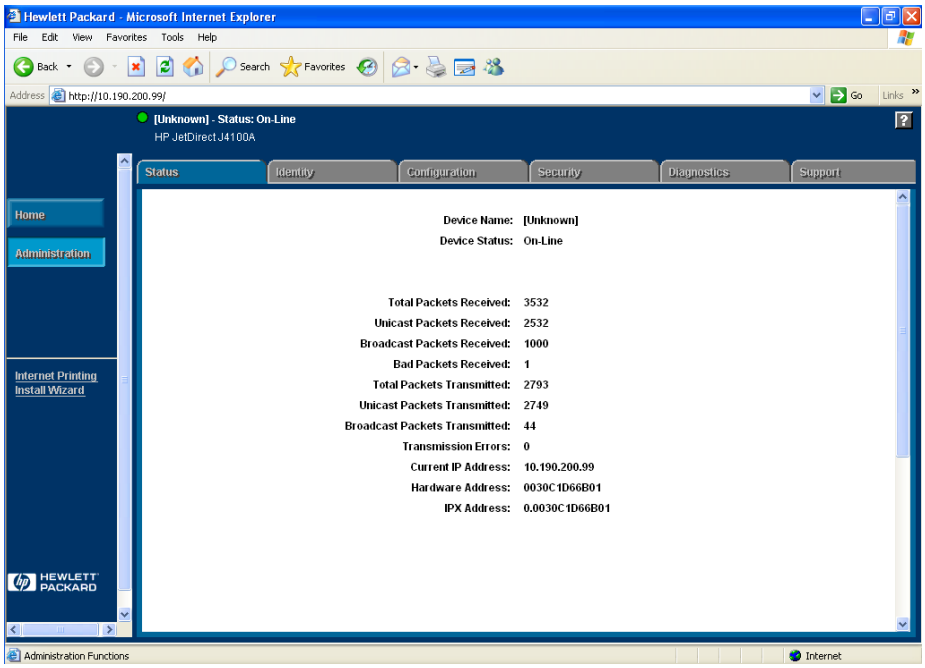
The Agilent Technologies 1260 LC must have been given a valid IP address via the BOOTP server.

In a web browser (Internet explorer for example) from the Acquisition server, type the IP address of the HPLC chain, in the address field. If the Internet browser is configured with a proxy server, it is mandatory to enter the IP address of the HPLC chain in the exceptions list. The following screen will be displayed.

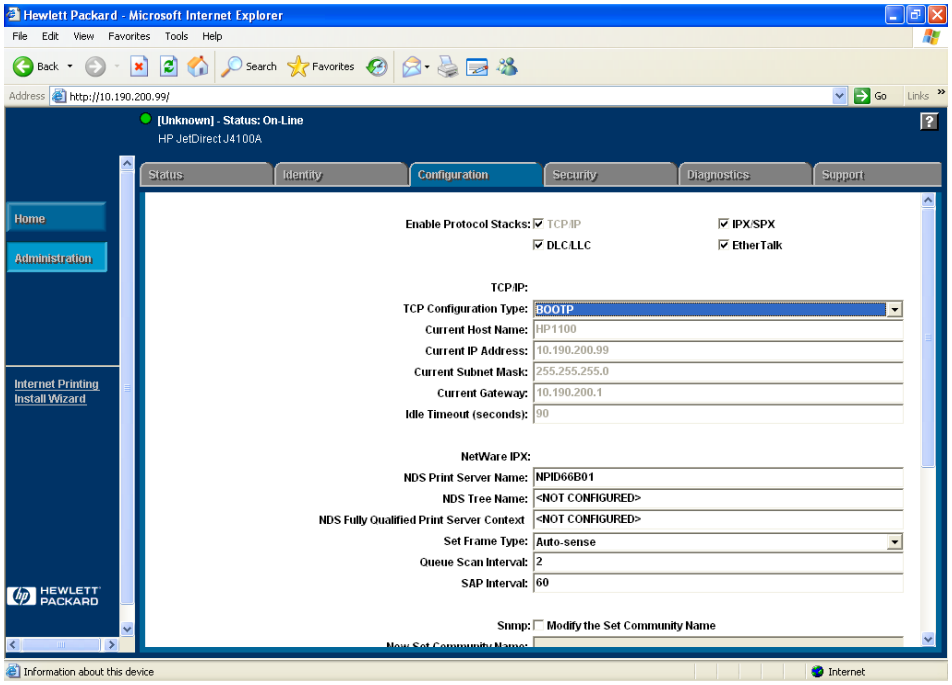


Click on the

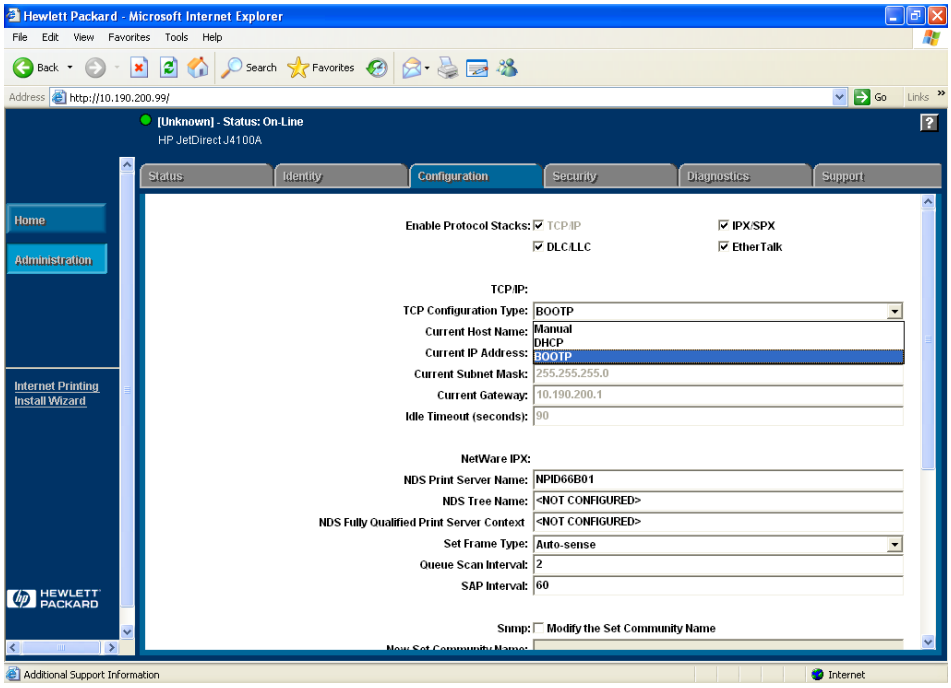
button on the left of the screen.



Click on the Configuration tab.

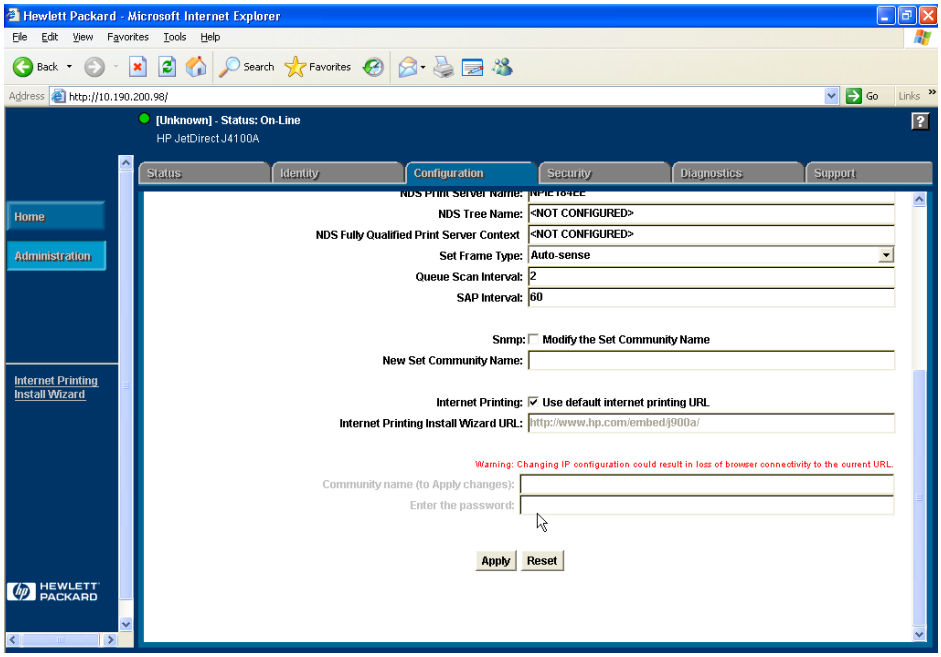


Select Manual in the *TCP Configuration Type* dropdown list.



Type the desired IP address, subnet mask and Gateway in the corresponding fields.

Finally, scroll down to the bottom of the screen and press the Apply button.


Hewlett Packard - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites
Address http://10.190.200.98/
Go Links
[Unknown] - Status: On-Line
HP JetDirect J4100A
Status Identity Configuration Security Diagnostics Support
Home
Administration
Internet Printing Install Wizard
HEWLETT PACKARD
NDS Tree Name: <NOT CONFIGURED>
NDS Fully Qualified Print Server Context <NOT CONFIGURED>
Set Frame Type: Auto-sense
Queue Scan Interval: 2
SAP Interval: 60
Snmp: Modify the Set Community Name
New Set Community Name:
Internet Printing: Use default internet printing URL
Internet Printing Install Wizard URL: http://www.hp.com/embedj900a/
Warning: Changing IP configuration could result in loss of browser connectivity to the current URL.
Community name (to Apply changes):
Enter the password:
Apply Reset

Reboot the HPLC chain.

For more details, please refer to the Agilent Technologies G1369A LAN Interface User Manual.

CompassCDS
Automating Retention Time and Timed Event Updating using the IntelliUpdate Function White Paper

Scion Instruments
1 Bain Square
Livingston, EH547DQ
United Kingdom

©Scion Instruments 2017
Publication Number BR501619
Revision A

Contents

Abstract 3
Introduction 3
Automatically changing instrument flow rate to correct of changes in chromatographic retention time 3
Use of reference peaks to correct for chromatographic variations 4
The CompassCDS IntelliUpdate feature 5
The CompassCDS IntelliUpdate feature and timed peak processing events 5
The CompassCDS Update Ratio function 7
Manually applying IntelliUpdate with the Update Ratio function 8
Conclusions 8

Abstract

Chromatographic column ageing as well as other instrumental and chemical effects can cause peak retention times to vary over time from the original values set in a method. Various approaches have been used to compensate for these variations including changing instrument control parameters such as carrier gas flow rate and using reference peaks to adjust the target retention times. However, none of these approaches can be used to adjust both the peak retention time targets and timed peak processing events on the chromatogram where these deviations occur. The CompassCDS IntelliUpdate feature can be used to automatically correct both retention times and timed events on chromatograms where such deviations occur.

Introduction

Changes in chromatographic retention times can be caused by both random factors like changes in injection technique or unexpected components in particular samples as well as systemic factors including gradual column ageing and small instrumental parameter changes such as leaks in either the HPLC or GC system.

There are several approaches that can be used to compensate for such changes. One is to simply replace the column if it is determined that this is the root cause of the problem. If a column has been in service for a long time and is demonstrating deteriorating in the form of gradually decreasing peak retention times, this would be a good solution. However, in order to achieve this, the system must be shut down, the column replaced and the system re-equilibrated.

This cannot be done during a series of automated runs. It also usually requires a certain level of expertise and could be disruptive to a routine laboratory's workflow. Also, it may be that the column is not the source of the problem.

Automatically changing instrument flow rate to correct of changes in chromatographic retention time

An alternative to replacing the column is to incrementally increase the flow rate of carrier gas for GC or mobile phase for HPLC. When applied to GC, this is termed Retention Time Locking or RTL. This can be done during a series of automated runs without operator intervention. However, this approach can have several limitations.

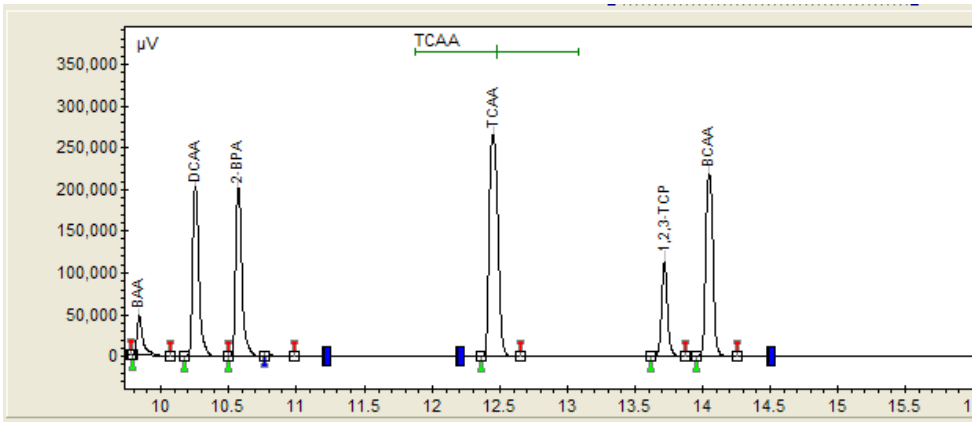
- The correction can only be made on the next run. When the problem is detected on a particular analysis, the instrumental parameters will be adjusted for the next run. If this was a problem specific to one injection or one sample, the correction will be made for the wrong injection.
- Increasing the flow rate can cause changes in the chromatographic characteristics because the Van Deempter curve is not constantly proportional to flow rate. Usually as the flow rate of the carrier in either HPLC or GC is increased, the resolving power of the column is decreased. This could lead to changes in resolution.

- This approach actually changes the analytical method and, if this is a validated method, the new method may have to have an abbreviated validation procedure, especially if the initial validation highlighted a limited flow rate range for the method.
- This approach is difficult to apply to HPLC. For gradient HPLC increasing or decreasing the flow rate changes the nature of the gradient.
- This approach can only be used on a few, vendor specific chromatographic instruments under the direct control of the data system.

Use of reference peaks to correct for chromatographic variations

It is far better to address changes in peak retention characteristics of a chromatogram through chromatographic peak processing. Using software, each chromatogram can be treated individually to correct for retention time variations. Usually these issues can be corrected for simply by the use of one or more reference peaks. Reference peaks are easily identifiable peaks, usually larger than most of the peaks in the chromatogram and, whenever possible, well resolved from other peaks. They are usually set to have a larger detection time window for than the other peaks. When a reference peak is detected at a time earlier or later than expected, the target retention times for the identification of other peaks around the reference peak are adjusted proportionally.

For example, if a reference peak is detected at a retention time 5% earlier than expected, the target retention times of the other peaks in the chromatogram are adjusted to be 5% earlier than the time reflected in the peak table. Normally, this adjustment is done for that run only and does not affect the retention times listed in the peak identification table which remain unchanged.



Reference Peaks | Retention Index | Identification using index

Peak Name	RT [min]	Abs.Window[mi	Window %	Cal.	Ref?	Mode
CAA	7.61	0.10	0.00	☑	☐	First
BAA	9.86	0.10	0.00	☑	☐	Nearest
DCAA	10.27	0.20	0.00	☑	☐	Nearest
2-BPA	10.59	0.20	0.00	☑	☐	Nearest
TCAA	12.48	0.60	0.00	☑	☑	Max. height
1,2,3-TCP	13.75	0.20	0.00	☑	☐	Nearest
BCAA	14.08	0.20	0.00	☑	☐	Nearest
DBAA	18.48	0.20	0.00	☑	☐	Nearest
2,3-DBPA	21.95	0.20	0.00	☑	☐	Nearest

Figure 1 CompassCDS Retention Time Reference Peak Input.

In Figure 1, the peak labeled TCAA is designated as a reference peak. Its retention time window has been expanded to +/- 0.6 minutes to make it easier to identify if the chromatography has hanged. The peak identified as TCAA will be the peak with the largest height in this retention time window.

The CompassCDS IntelliUpdate feature

While reference peaks can be used to correct for random chromatographic variation, systemic variations can be a more serious problem. Column retention time characteristics can change over time. This is sometimes termed column ageing. As columns age, the retention times of the reference peaks can migrate beyond the pre-set time windows. These changes usually occur gradually but during the analysis of an extended series of samples, can be quite significant.

CompassCDS can utilize such gradual changes to constantly adjust target retention times and thereby ensure ongoing, accurate peak identification.

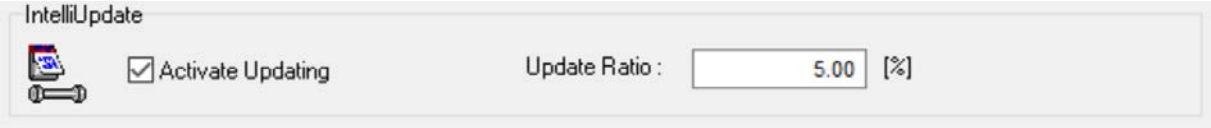


Figure 2 CompassCDS IntelliUpdate Ratio parameter

When the IntelliUpdate feature is activated in CompassCDS, as shown in Figure 3, the Update Ratio percentage is used to change the retention times in the peak table for both the reference and non-reference peaks. If a reference peak is detected 1% earlier than expected then all of the retention times in the analytical method peak table are decreased by 1%. In this way even a significantly larger gradual change in retention time (for example 10%) can be corrected by the IntelliUpdate function. Proper peak identification can be maintained even after significant changes in the chromatography.

The CompassCDS IntelliUpdate feature and timed peak processing events

Adjusting only peak retention time targets is not enough as timed events, which are used to maintain proper peak processing, must also be adjusted to correspond to the adjusted peak retention times. Without this adjustment, improper peak processing will give incorrect results.

The CompassCDS IntelliUpdate feature will also automatically adjust timed events so that proper peak processing is maintained throughout each run.

As the retention time for a peak decreases, for example 5% as shown in Table 1, the CompassCDS IntelliUpdate feature can adjust the times for the timed events in the integration table 5%. Importantly, the modified times are used for peak processing on the chromatogram where the change in the reference peak retention time occurred and not just on the subsequent run.

Table 1 CompassCDS IntelliUpdate adjusts expected peak retention times and timed events

Event	Original times	Time offset for reference peaks	New times
Retention time of reference peak	8.7	5% earlier	8.27
Horizontal forward start	6.8	5% earlier	6.46
Horizontal forward stop	8.2	5% earlier	7.79
Horizontal forward next peak start	8.4	5% earlier	7.98
Horizontal forward next peak stop	9.2	5% earlier	8.74

The effect of timed event adjustment is shown in Figure 3 below. In this example, the retention times of all of the peaks including the reference peak Pentachlorobenzene have become 5% shorter. In the lower chromatogram, the CompassCDS column ageing factor was turned off.

The peak processing times events (shown in the figure) were maintained at the original times. Here the carefully chosen timed events do not function properly because they are being executed at the original and now incorrect times.

The timed events in the upper chromatogram have been automatically adjusted in the timed events table by the CompassCDS IntelliUpdate feature to be 5% shorter. These now execute at the correct time relative to the peaks in the actual chromatogram giving the correct peak processing and the correct results.

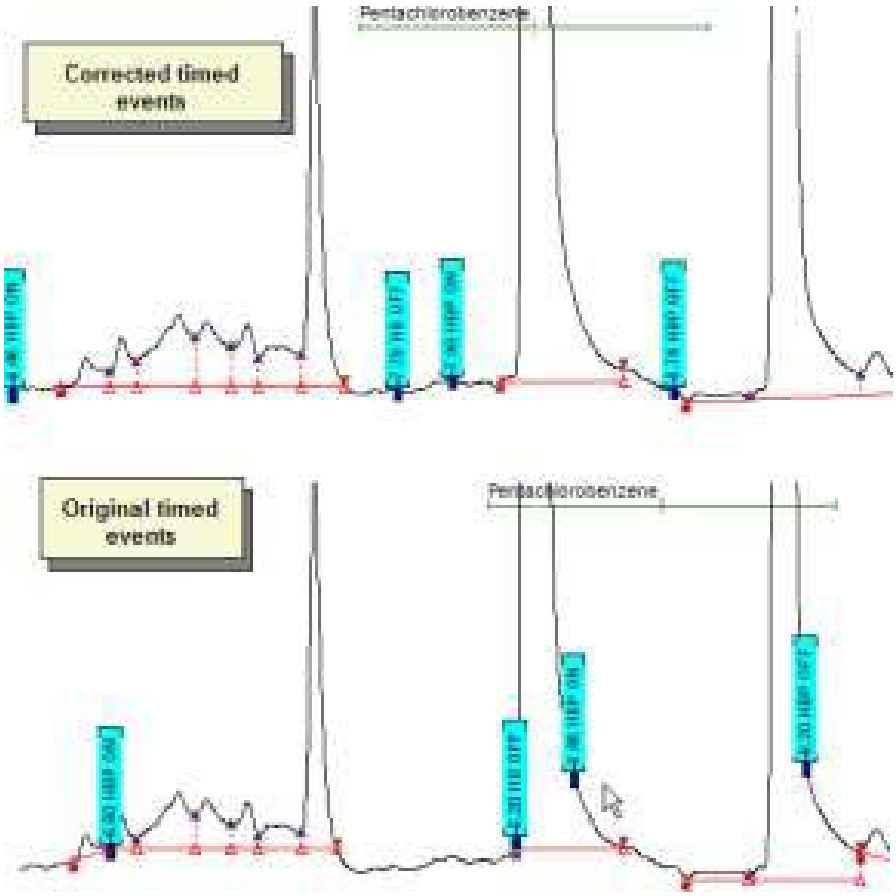


Figure 3 CompassCDS IntelliUpdate adjusts timed events

The CompassCDS Update Ratio function

Although column ageing and instrument variation problems can result in changes in chromatography, now and again, individual samples can also cause significant retention time shifts. These changes may often only occur with one anomalous sample and then the chromatography returns to normal. If retention times and timed events were to be changed by a large amount, based on such an outlier chromatogram, subsequent chromatograms could be incorrectly processed. The CompassCDS IntelliUpdate feature can be used to adjust for this possibility. The Update Ratio (entry value shown in Figure 2) determines how rapidly CompassCDS will react to sudden changes in the retention times of the reference peaks. This ratio determines how much of an adjustment of retention time targets and timed events is done due to the effect of any one chromatogram.

The effect of a ratio of 25% is shown in Figure 4. Here the change in retention time of the reference peak in chromatogram 6 only causes a small change in the timed events and peak identification table. This entry allows CompassCDS to successfully adjust to gradual changes in retention times but not to over react to “one of a kind” events.

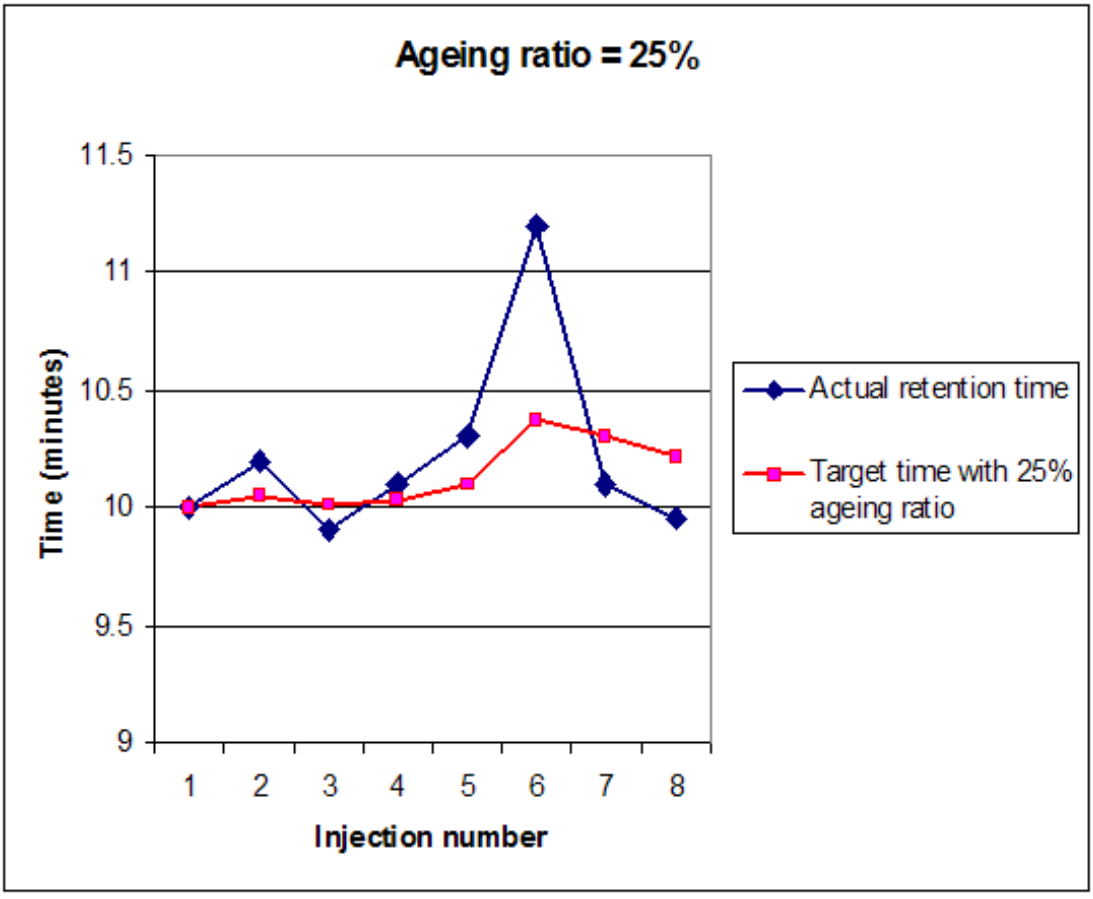


Figure 4 Effect of CompassCDS Update Ratio when one of a kind sample effects are detected.

Manually applying IntelliUpdate with the Update Ratio function

Sometimes, automating changes to retention times in the peak identification or timed events table might be considered unwise. It may be better for chemist to first assess the chromatograms before any changes are made. In such cases, the CompassCDS column IntelliUpdate makes implementing these changes easier. If the chemist determines that the changing chromatogram warrants changes to the peak and timed events table, a new chromatogram can be run with IntelliUpdate turned on and the Update Ratio set to 100%. All of the tables will be updated accurately without the possibility of missing a peak or event.

Conclusions

The CompassCDS IntelliUpdate feature meets all of the criteria required for successfully compensating for variation in retention time originating from any source.

- Fully automatic
- Can be used on any LC/GC system, even those not being controlled by CompassCDS software
- Does not require re-validation of an analytical method as the instrument control parameters are not modified.
- Uses the commonly accepted reference peak method to determine the amount of change in peak retention time from injection to injection.
- Corrects timed peak processing events so that peak are not only identified correctly but they are also processed correctly
- Can be set to minimize the “correction” due to unique sample based variations
- Can be used in either manual or automatic mode.

CompassCDS IntelliUpdate minimizes the effect of column

CompassCDS Software End User License Agreement

Important: Please carefully read the License Agreement below before installing the software product. The right to use the software product which accompanies this Agreement (the "Software") is provided only on the condition that you agree to this Agreement. If you do not agree to the terms of this Agreement, you may not install the Software and you may return the package for a full refund. However, installing the Software indicates your acceptance of this Agreement.

In return for payment of the one-time license fee for the Software, you receive from Scion Instruments a license to use the Software subject to the following terms and conditions:

1. The Software may be used without time limit on one personal computer or workstation.
2. A separate license agreement and fee is required for each personal computer or workstation on which the Software is used.
3. The Software may not be duplicated or copied except for archive purposes, program error verification, or to replace defective media, and all copies made must bear the copyright notices contained in the original.
4. This license and the Software may be transferred to a third party only with the prior written consent of Scion Instruments, provided the third party agrees to all terms of this Agreement and you do not retain any copies of the Software.
5. Purchase of this license does not transfer any right, title or interest in the Software to you except as specifically set forth in this Agreement. You are on notice that the Software is protected under various domestic and international copyright laws and treaties.
6. Scion Instruments reserves the right to terminate this Agreement by notice to you upon breach of this Agreement by you. In the event of termination, you will either return all copies of the Software to Scion Instruments or, with prior consent from Scion Instruments, provide Scion Instruments with a certificate of destruction of all copies.
7. In the event you modify the Software or include it in any other software program, upon termination of this Agreement you will either remove the Software or any portion thereof from the modified program and return it to Scion Instruments or provide Scion Instruments with a certificate of destruction therefor.

© Scion Instruments 2017
Publication Number BR501622
Revision A

Limited Warranty

Software: Scion Instruments warrants for a period of ninety (90) days from the date of purchase that the Software will execute its programming instructions when properly installed on the personal computer or workstation indicated on this package. Scion Instruments does not warrant that the operation of the Software will be uninterrupted or error free. In the event that the Software fails to execute its programming instructions during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Software and all copies.

Media: Scion Instruments warrants the media upon which the Software is recorded to be free from defects in materials and workmanship under normal use for a period of ninety (90) days from the day of purchase. In the event any media prove to be defective during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Software and all copies.

Notice of warranty claims: You must notify Scion Instruments in writing of any warranty claim not later than the expiration of the warranty period.

LIMITATIONS OF WARRANTY: SCION INSTRUMENTS MAKES NO OTHER EXPRESS WARRANTY, WHETHER WRITTEN OR ORAL, WITH RESPECT TO THE SOFTWARE. ANY IMPLIED WARRANTY OF MERCHANTABILITY OR FITNESS IS LIMITED TO THE 90-DAY DURATION OF THIS LIMITED WARRANTY. SOME STATES DO NOT ALLOW LIMITATIONS ON HOW LONG AN IMPLIED WARRANTY LASTS, SO THE ABOVE LIMITATION OR EXCLUSION MAY NOT APPLY TO YOU.

This warranty gives specific legal rights, and you may also have other rights, which vary from state to state.

EXCLUSIVE REMEDIES: THE REMEDIES PROVIDED ABOVE ARE YOUR SOLE AND EXCLUSIVE REMEDIES. IN NO EVENT SHALL SCION INSTRUMENTS BE LIABLE FOR ANY DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES (INCLUDING LOST PROFIT) WHETHER BASED ON WARRANTY, CONTRACT, TORT, OR ANY OTHER LEGAL THEORY. SOME STATES DO NOT ALLOW THE EXCLUSION OR LIMITATION OF INCIDENTAL OR CONSEQUENTIAL DAMAGES, SO THE ABOVE LIMITATIONS OR EXCLUSIONS MAY NOT APPLY TO YOU.

Warranty Service: Warranty service may be obtained from the nearest Scion Instruments sales office or other location indicated in the user manual.

© Scion Instruments 2017
Publication Number BR501622
Revision A

CompassCDS Control Driver Software
End User License Agreement

Important: Please carefully read the End User License Agreement below before installing this CompassCDS Control Driver software product. The right to use the CompassCDS Control Driver software product which accompanies this Agreement (the "Driver Software") is provided only on the condition that you agree to abide by the terms of this Agreement. If you do not agree to abide by the terms of this Agreement, you may not install the Driver Software and you may return the package for a full refund. However, installing the Driver Software indicates your acceptance of this Agreement.

In return for payment of the one-time license fee for the Driver Software, you receive, from Scion Instruments, a license to use the Driver Software subject to the following terms and conditions:

1. The Driver Software may be installed and used without time limit on one standalone workstation, or if configured as a client server network, on the server and all CompassCDS network client computers.

2. The Driver Software license is considered to be a “site” license when installed with CompassCDS in client server configurations and as such, can be installed on the server and all CompassCDS client computers without the requirement for additional control driver license fees for each individual computer. A “site” is defined as a CompassCDS server or collection of servers and all connected CompassCDS client computers located at the same physical address. A “site” can include one or more laboratories or offices locations at the same physical address.

3. The Driver Software may not be duplicated or copied except for archive purposes, program error verification, or to replace defective media, and all copies made must bear the copyright notices contained in the original.

4. This license and the Driver Software may be transferred to a third party only with the prior written consent of Scion Instruments, provided the third party agrees to all terms of this Agreement and you do not retain any copies of the Driver Software.

5. Purchase of this license does not transfer any right, title or interest in the Driver Software to you except as specifically set forth in this Agreement. You are on notice that the Driver Software is protected under various domestic and international copyright laws and treaties.

6. Scion Instruments reserves the right to terminate this Agreement by notice to you upon breach of this Agreement by you. In the event of termination, you will either return all copies of the Driver Software to Scion Instruments or, with prior consent from Scion Instruments, provide Scion Instruments with a certificate of destruction of all copies.

7. In the event that you modify the Driver Software or include it in any other software program, upon termination of this Agreement, you will either remove the Driver Software or any portion thereof from the modified program and return it to Scion Instruments or provide Scion Instruments with a certificate of destruction therefor.

© Scion Instruments 2017
Publication Number BR501623
Revision A

Limited Warranty

Driver Software: Scion Instruments warrants for a period of one (1) Year from the date of purchase that the Driver Software will execute its programming instructions when properly installed on a standalone workstation, network server or network client computer that conforms to the minimum required hardware specifications and approved operating systems. Scion Instruments does not warrant that the operation of the Driver Software will be uninterrupted or error free. In the event that the Driver Software fails to execute its programming instructions during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Driver Software and all copies.

Media: Scion Instruments warrants the media upon which the driver Software is recorded to be free from defects in materials and workmanship under normal use for a period of one (1) Year from the day of purchase. In the event any media prove to be defective during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Software and all copies.

Notice of warranty claims: You must notify Scion Instruments, in writing, of any warranty claim not later than the expiration of the warranty period.

LIMITATIONS OF WARRANTY: SCION INSTRUMENTS MAKES NO OTHER EXPRESS WARRANTY, WHETHER WRITTEN OR ORAL, WITH RESPECT TO THE DRIVER SOFTWARE. ANY IMPLIED WARRANTY OF MERCHANTABILITY OR FITNESS IS LIMITED TO THE ONE (1) YEAR DURATION OF THIS LIMITED WARRANTY. SOME STATES DO NOT ALLOW LIMITATIONS ON HOW LONG AN IMPLIED WARRANTY LASTS, SO THE ABOVE LIMITATION OR EXCLUSION MAY NOT APPLY TO YOU.

This warranty gives specific legal rights, and you may also have other rights, which vary from state to state.

EXCLUSIVE REMEDIES: THE REMEDIES PROVIDED ABOVE ARE YOUR SOLE AND EXCLUSIVE REMEDIES. IN NO EVENT SHALL SCION INSTRUMENTS BE LIABLE FOR ANY DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES (INCLUDING LOST PROFIT) WHETHER BASED ON WARRANTY, CONTRACT, TORT, OR ANY OTHER LEGAL THEORY. SOME STATES DO NOT ALLOW THE EXCLUSION OR LIMITATION OF INCIDENTAL OR CONSEQUENTIAL DAMAGES, SO THE ABOVE LIMITATIONS OR EXCLUSIONS MAY NOT APPLY TO YOU.

Warranty Service: Warranty service may be obtained from the nearest Scion Instruments sales office or other location indicated in the user manual.

© Scion Instruments 2017
Publication Number BR501623
Revision A

Agilent 1260 Control Driver Software
End User License Agreement

Important: Please carefully read the End User License Agreement below before installing this Agilent 1260 Control Driver software product. The right to use the Agilent 1260 Control Driver software product which accompanies this Agreement (the "Driver Software") is provided only on the condition that you agree to abide by the terms of this Agreement. If you do not agree to abide by the terms of this Agreement, you may not install the Driver Software and you may return the package for a full refund. However, installing the Driver Software indicates your acceptance of this Agreement.

In return for payment of the one-time license fee for the Driver Software, you receive, from Scion Instruments, a license to use the Driver Software subject to the following terms and conditions:

1. The Driver Software may be installed and used without time limit on one instrument.
2. A separate license agreement and fee is required for each instrument on which the Control Driver Software is used.
3. The Driver Software may not be duplicated or copied except for archive purposes, program error verification, or to replace defective media, and all copies made must bear the copyright notices contained in the original.
4. This license and the Driver Software may be transferred to a third party only with the prior written consent of Scion Instruments, provided the third party agrees to all terms of this Agreement and you do not retain any copies of the Driver Software.
5. Purchase of this license does not transfer any right, title or interest in the Driver Software to you except as specifically set forth in this Agreement. You are on notice that the Driver Software is protected under various domestic and international copyright laws and treaties.
6. Scion Instruments reserves the right to terminate this Agreement by notice to you upon breach of this Agreement by you. In the event of termination, you will either return all copies of the Driver Software to Scion Instruments or, with prior consent from Scion Instruments, provide Scion Instruments with a certificate of destruction of all copies.
7. In the event that you modify the Driver Software or include it in any other software program, upon termination of this Agreement, you will either remove the Driver Software or any portion thereof from the modified program and return it to Scion Instruments or provide Scion Instruments with a certificate of destruction therefor.

© Scion Instruments 2017
Publication Number BR501624
Revision A

Limited Warranty

Driver Software: Scion Instruments warrants for a period of one (1) Year from the date of purchase that the Driver Software will execute its programming instructions when properly installed on a standalone workstation, network server or network client computer that conforms to the minimum required hardware specifications and approved operating systems. Scion Instruments does not warrant that the operation of the Driver Software will be uninterrupted or error free. In the event that the Driver Software fails to execute its programming instructions during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Driver Software and all copies.

Media: Scion Instruments warrants the media upon which the driver Software is recorded to be free from defects in materials and workmanship under normal use for a period of one (1) Year from the day of purchase. In the event any media prove to be defective during the warranty period, your remedy shall be to return the media to Scion Instruments for replacement. Should Scion Instruments be unable to replace the media within a reasonable amount of time, your alternate remedy shall be a refund of the purchase price upon return of the Software and all copies.

Notice of warranty claims: You must notify Scion Instruments, in writing, of any warranty claim not later than the expiration of the warranty period.

LIMITATIONS OF WARRANTY: SCION INSTRUMENTS MAKES NO OTHER EXPRESS WARRANTY, WHETHER WRITTEN OR ORAL, WITH RESPECT TO THE DRIVER SOFTWARE. ANY IMPLIED WARRANTY OF MERCHANTABILITY OR FITNESS IS LIMITED TO THE ONE (1) YEAR DURATION OF THIS LIMITED WARRANTY. SOME STATES DO NOT ALLOW LIMITATIONS ON HOW LONG AN IMPLIED WARRANTY LASTS, SO THE ABOVE LIMITATION OR EXCLUSION MAY NOT APPLY TO YOU.

This warranty gives specific legal rights, and you may also have other rights, which vary from state to state.

EXCLUSIVE REMEDIES: THE REMEDIES PROVIDED ABOVE ARE YOUR SOLE AND EXCLUSIVE REMEDIES. IN NO EVENT SHALL SCION INSTRUMENTS BE LIABLE FOR ANY DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES (INCLUDING LOST PROFIT) WHETHER BASED ON WARRANTY, CONTRACT, TORT, OR ANY OTHER LEGAL THEORY. SOME STATES DO NOT ALLOW THE EXCLUSION OR LIMITATION OF INCIDENTAL OR CONSEQUENTIAL DAMAGES, SO THE ABOVE LIMITATIONS OR EXCLUSIONS MAY NOT APPLY TO YOU.

Warranty Service: Warranty service may be obtained from the nearest Scion Instruments sales office or other location indicated in the user manual.

© Scion Instruments 2017
Publication Number BR501623
Revision A